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Conjectured enumeration of Vassiliev invariants

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Abstract A rational Ansatz is proposed for the generating function $\sum_{j,k}\beta_{2j+k,2j}x^jy^k$, where $\beta_{m,u}$ is the number of primitive chinese character diagrams with u univalent and $2m-u$ trivalent vertices. For $P_m := \sum_{u\geq 2}\beta_{m,u}$, the conjecture leads to the sequence

$$1,1,1,2,3,5,8,12,18,27,39,55,\underline{78,108,150,207,284,388,532,726}$$

for primitive chord diagrams of degrees $m\leq 20$, with predictions underlined. The asymptotic behaviour $\lim_{m\to\infty}P_m/r^m = 1.06260548918755$ results, with $r = 1.38027756909761$ solving $r^4 = r^3+1$. Vassiliev invariants of knots are then enumerated by

$$0,1,1,3,4,9,14,27,44,80,132,232,\underline{384,659,1095,1851,3065,5128,8461,14031}$$

and Vassiliev invariants of framed knots by

$$1,2,3,6,10,19,33,60,104,184,316,548,\underline{932,1591,2686,4537,7602,12730,21191,35222}$$

These conjectures are motivated by successful enumerations of irreducible Euler sums. Predictions for $\beta_{15,10}$, $\beta_{16,12}$ and $\beta_{19,16}$ suggest that the action of sl and osp Lie algebras, on baguette diagrams with ladder insertions, fails to detect an invariant in each case.

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1 Introduction

The purpose of this note is to report a conjectured enumeration of Vassiliev invariants [1], which results from fits to the data of [2, 3, 4] on the enumeration of primitive chinese character diagrams. It is motivated by recent successes [5, 6] of conjectured enumerations [7] of irreducible multiple zeta values (MZVs) [8, 9, 10] and their extensions, alternating Euler sums [11, 12]. It is consistent with all 64 proven results [3] and lower bounds [4] on the bigrading of chinese characters by degree, $m \leq 14$, and number of univalent vertices, $u = 2j \leq m$. Moreover, it saturates the bounds for $m = 13, 14$. For $m \geq 15$, some lower bounds are exceeded by the Ansatz, suggesting invariants that were not detected by Lie algebras of type sl and osp operating on a restricted set of diagrams.

A chinese character diagram of degree m, with u univalent vertices, has $2m-u$ trivalent vertices. If the univalent vertices are attached to a circle, representing a closed Wilson line, the resultant graph has $m+1$ loops, when regarded as a Feynman diagram in the perturbative expansion of a topological quantum field theory [13, 14]. In abstracting from the notion of a topological field theory, Dror Bar–Natan was led to the consideration of weight systems [14]. Combinatorical investigation of such weight systems enables an enumeration of Vassiliev invariants for knots, via the equivalence proven in [2, 15, 16].

The data of [2, 3] concern the number, $\beta_{m,u}$, of diagrams that cannot be reduced merely by the application of the antisymmetry and Jacobi relations (called AS and IHX relations in [2]) that obtain when structure constants of a Lie algebra are associated with the vertices of a chinese character. The numbers so obtained classify the dimensionality of the naturally graded spaces of primitive elements in the bialgebra established by weight systems [2]. Summing over $u \geq 2$, one obtains an enumeration of connected chord diagrams, modulo four-term relations, which is equivalent to an enumeration of primitive Vassiliev invariants by [2]

$$P_m := \sum_{u\geq 2} \beta_{m,u}\,. \tag{1}$$

These, in turn, generate the numbers, V_m and F_m, of Vassiliev invariants of knots and framed knots, respectively, via the Euler transforms

$$\prod_{m\geq 2}(1-y^m)^{-P_m} = 1 + \sum_{m\geq 2} V_m y^m\,, \tag{2}$$

$$\prod_{m\geq 1}(1-y^m)^{-P_m} = 1 + \sum_{m\geq 1} F_m y^m\,, \tag{3}$$

with $P_1 = \beta_{1,2} = 1$ implying that $V_{m+1} = F_{m+1} - F_m$.

It is known [17] that at some degree, $m > 12$, one will eventually encounter structure more general than that spanned by Lie algebras. Recently [18] it was shown that a Lie superalgebra detects structure at $m = 19$ and $u = 4$ that is not detected by semisimple Lie algebras. Moreover, even superalgebras are proven to be insufficient, in the long run [17].

As a contribution to such studies, we here attempt to infer, from existing data [3, 4], a closed rational form for the generator

$$b(x,y) := \sum_{j,k\geq 0} (\beta_{2j+k,2j} - 1) x^j y^k\,. \tag{4}$$

Assuming that Vassiliev invariants fail to distinguish a knot from its mirror image we set $\beta_{m,2j+1} = 0$. Then, with $P_1 = \beta_{1,2} = \beta_{0,0} = 1$, we conjecture the sequences generated by (1,2,3). The key ingredient is the hypothesis of common features in the generators for primitive Vassiliev invariants and for irreducible MZVs and Euler sums.

Like the chinese character diagrams of [2], the MZVs of [8] and the Euler sums of [11] have a bigrading. In the case of MZVs and Euler sums, it is by weight w and depth d. The distinctive prediction of the conjecture of [7] is that the number, $D_{w,d}$, of irreducible MZVs is generated by a pseudopolynomial at any fixed depth. In other words, the generating function $\sum_j D_{2j+3d,d}x^j$ is believed to have singularities only at roots of unity, for fixed d.

The clue that the enumerations of MZVs and Vassiliev invariants might be akin comes from the Kontsevich integral [15], which is a universal knot invariant, corresponding to the holonomy of the flat Knizhnik-Zamolodchikov connection [19, 20]. It thus evaluates in terms of MZVs, in a natural manner [21]. Moreover Dirk Kreimer, the present author and coworkers have accumulated abundant evidence [22]–[29] that knots and MZVs are connected via the counterterms of quantum field theory. These counterterms have recently been construed [30] as deriving from the antipode of a quasi-Hopf algebra, whose failure to be coassociative may be controlled by a Drinfeld associator [20, 21], specific to the quantum field theory in question. One is thus encouraged to fit the recent [3] bigraded data on chinese characters with pseudopolynomial generating functions, deriving from an underlying rational generator in (4). This was surprisingly easy to achieve, and quickly suggested a closed form for the rational generator.

Section 2 gives a detailed analysis of the data [2, 3] on $\beta_{m,u}$, leading to pseudopolynomial generators for fixed values of $m-u$ or $u=2j$. In Section 3 these observations are subsumed into a relatively simple Ansatz that fits all available data and satisfies all known bounds. Section 4 gives comments and conclusions.

2 Analysis of data

The impressive progress reported by Jan Kneissler in [3] extended the results on $\beta_{m,u}$ from degrees $m \leq 9$, achieved in [2], up to $m \leq 12$. All values of $\beta_{m,u}$ with $m \leq 12$ are known, save $\beta_{12,0}$, which is merely bounded from below. In addition to these, one knows that [2]

$$\begin{aligned}\beta_{m,0} &= \beta_{m+1,2}\,, &(5)\\ \beta_{2j,2j} &= 1\,, &(6)\\ \beta_{2j+1,2j} &= \left\lfloor\frac{j+3}{3}\right\rfloor\,, &(7)\end{aligned}$$

where $\lfloor x \rfloor$ denotes the largest integer that does not exceed x.

Moreover, there exist lower bounds, obtained by a ‘thickening’ procedure [2] that enumerates the invariants detected by sl and osp Lie algebras. Restricting attention to diagrams generated by ladder insertions in baguette [31] diagrams (called caterpillar diagrams in [3]) lower bounds on $\beta_{m,u}$ were obtained in [4] for $20 \geq m \geq 13$. With $u=2$, further invariants were found for $20 \geq m \geq 14$. The values in Table 1 that are lower bounds are indicated by underlining. The Ansatz adduced in Section 3 saturates these.

Table 1: Values and <u>lower bounds</u> for $\beta_{m,u}$ with $m \le 14$.

	$u=0$	$u=2$	$u=4$	$u=6$	$u=8$	$u=10$	$u=12$	$u=14$
$m=\ 0$	1							
$m=\ 1$	1	1						
$m=\ 2$	1	1						
$m=\ 3$	1	1						
$m=\ 4$	2	1	1					
$m=\ 5$	2	2	1					
$m=\ 6$	3	2	2	1				
$m=\ 7$	4	3	3	2				
$m=\ 8$	5	4	4	3	1			
$m=\ 9$	6	5	6	5	2			
$m=10$	8	6	8	8	4	1		
$m=11$	9	8	10	11	8	2		
$m=12$	$\underline{11}$	9	13	15	12	5	1	
$m=13$	$\underline{13}$	$\underline{11}$	$\underline{16}$	$\underline{20}$	$\underline{18}$	$\underline{10}$	3	
$m=14$	$\underline{15}$	$\underline{13}$	$\underline{19}$	$\underline{25}$	$\underline{26}$	$\underline{17}$	7	1

The possibility of a simple enumeration of Vassiliev invariants was suggested by observing that Oliver Dasbach's result [32] for the third diagonal of Table 1, namely

$$\beta_{2j+2,2j} = \left\lfloor \frac{(j+3)^2+3}{12} \right\rfloor , \tag{8}$$

is echoed by a simple fit to the first two columns of Table 1, namely

$$\beta_{m,0} - 1 = \beta_{m+1,2} - 1 \stackrel{?}{=} \left\lfloor \frac{(m-1)^2+3}{12} \right\rfloor , \tag{9}$$

which is proven for $11 \ge m \ge 0$. This conjecture[1] was lodged as A014591 in Neil Sloane's encyclopedia of integer sequences [34], prior to the lower bounds of [4] for $\beta_{m,0}$ with $19 \ge m \ge 12$. It was then found to saturate these lower bounds for $16 \ge m \ge 12$. Having thus fitted 12 data and saturated a further 5 bounds, we suggest that the lower bounds of [4] for $\beta_{m,0}$ are exceeded for $m = 17, 18, 19$, in accordance with (9).

Encouraged by results for the three leading diagonals of Table 1, and fits to its first two columns, we conjectured that the generator (4) has Taylor coefficients in x that are pseudopolynomials in y, with singularities at $y^2 = 1$ and $y^3 = 1$, and Taylor coefficients in y that are pseudopolynomials in x, with singularities at $x^2 = 1$ and $x^3 = 1$.

The guiding intuition behind this conjecture was the fact that the conjectured enumeration of MZVs in [7] had been seeded by singularities at square and cube roots of unity, with

$$\prod_{j\ge0}\prod_{d>0}(1-x^j y^d)^{D_{2j+3d,d}} \stackrel{?}{=} 1 - \frac{y}{1-x} - \frac{y^2}{1-x^2}\frac{y^2-x^3}{1-x^3} , \tag{10}$$

[1] Conjectured equalities are indicated by $\stackrel{?}{=}$, as in (9).

proposed [7] as the generator of the number, $D_{w,d}$, of irreducible MZVs of weight $w \geq 3d$ and depth d. This Ansatz was initially inferred from rather limited data. Subsequently, it has survived intensive testing. For example the prediction [7] $D_{23,7} = 4$ was confirmed [6] as the rank deficiency of the $447\,678 \times 74\,613$ matrix that results from the interplay of the weight-length [8, 21] and depth-length [12] shuffle algebras for MZVs. It is an outstanding puzzle to understand the third term in (10), which is absent in the enumeration

$$\prod_{j\geq 0}\prod_{d>0}(1-x^j y^d)^{M_{2j+3d,d}} \stackrel{?}{=} 1 - \frac{y}{1-x}\,, \tag{11}$$

for the number, $M_{w,d}$, of irreducible Euler sums of weight w and depth d that serve to reduce all MZVs. The difference between (10) and (11) first surfaces at weight $w = 12$, where $\zeta(4,4,2,2) := \sum_{k>l>m>n>0} k^{-4} l^{-4} m^{-2} n^{-2}$ is *not* reducible to MZVs of depth $d < 4$ but *is* reducible to the depth-2 alternating Euler sum [11] $\sum_{m>n>0}(-1)^{m+n} m^{-9} n^{-3}$, as anticipated [26] by the connection [22] between knots and numbers effected by the counterterms of quantum field theory.

Close study of Table 1 suggests that the enumeration of Vassiliev invariants, with $m - u \geq 3$, is *not* obtainable from that of irreducible MZVs by mere relabelling. This presumably reflects a difference in the Drinfeld associators controlling the failures of coassociativity in the quasi-Hopf algebras that relate to knot theory, in the case of rational-valued Vassiliev invariants [33], and to the Knizhnik-Zamolodchikov equation [19], in the case of irrational MZVs. However, the connections between knots and MZVs, effected by the Kontsevich integral [15] and by quantum field theory [22], lead us to expect resemblances between generating functions for these distinct structures.

Hence we sought to generate columns and diagonals of Table 1 with pseudopolynomials whose singularities occur only at square and cube roots of unity. With such limited pseudopolynomial singularities posited for

$$g_k(x) \;:=\; \sum_{j\geq 0} \beta_{2j+k,2j} x^j\,, \tag{12}$$

$$h_j(y) \;:=\; \sum_{k\geq 0} (\beta_{2j+k,2j} - 1) y^k\,, \tag{13}$$

it is apparent that the full generator (4) must have a denominator that involves a factor which couples x to y, in order to generate terms that are more singular at $x = 1$ when one expands to higher order in y, and vice versa.

Fortunately, the proven sequence [3]

$$1, 1, 1, 2, 3, 5, 8, 12, 18, 27, 39, 55 \tag{14}$$

for P_m, with $m \leq 12$, provided a clue as to this coupling, since the ratio of successive terms appears to tend to a value $r \approx 1.4$. An origin of such a ratio is not hard to imagine. Consider, for example, the number, $D_{3d,d}$, of irreducible MZVs of depth d and weight $w = 3d$, which is the lowest weight at which sums of this depth may exhibit irreducibility. Then from (10), at $x = 0$, one obtains

$$\prod_{d>0} \frac{1}{(1-y^d)^{D_{3d,d}}} \stackrel{?}{=} \frac{1}{1-y-y^4}\,, \tag{15}$$

which has been verified through $O(y^7)$, i.e. for weights $w = 3d \leq 21$, and is lodged as A020999 in [34]. The asymptotic growth is determined by the singularity of $1/(1-y-y^4)$ at $y = 1/r$, with $r = \lim_{d\to\infty} D_{3d+3,d+1}/D_{3d,d} = 1.38027756909761$ solving $1 = r^{-1} + r^{-4}$. Moreover, one can generate such an asymptotic growth in the case of (1), as follows.

Suppose that $b(x, y)$ in (4) had a singularity of the form $1/(1 - y - x^2)$. Then the summation in (1) would detect a $1/(1 - y - y^4)$ singularity from the term with $x = y^2$ in

$$p(y) := \sum_{m\geq 1}(P_m - 1)y^m = b(y^2, y) - b(0, y) + \frac{y^4}{(1-y)(1-y^2)}\,, \tag{16}$$

and hence give $\lim_{m\to\infty} P_{m+1}/P_m = r \approx 1.38$. Thus previous experience with MZVs, combined with a ratio test $r \approx 1.4$ from (14), led us to suspect a $1/(1-y-x^2)$ singularity in (4). Hence we expected that expanding in powers of y would lead to higher powers of $1/(1 - x^2)$ in (12), as k increases. This observation greatly facilitated the discovery of simple pseudopolynomial fits to the first few instances of (12), namely

$$g_0(x) = \frac{1}{1-x} = \sum_j D_{3+2j,1}x^j\,, \tag{17}$$

$$g_1(x) = \frac{g_0(x)}{1-x^3} = \sum_j D_{8+2j,2}x^j\,, \tag{18}$$

$$g_2(x) = \frac{g_1(x)}{1-x^2} = \sum_j (D_{11+2j,3} - D_{8+2j,2})x^{j-1}\,, \tag{19}$$

$$g_3(x) \stackrel{?}{=} \frac{g_2(x)}{1-x^2} + \frac{x}{(1-x^2)(1-x^3)}\,, \tag{20}$$

$$g_4(x) \stackrel{?}{=} \frac{g_3(x)}{1-x^2} + \frac{1}{1-x^3}\,, \tag{21}$$

$$g_5(x) \stackrel{?}{=} \frac{g_4(x)}{1-x^2} + \frac{x}{1-x^2}\,, \tag{22}$$

for the first 6 diagonals of Table 1. For the first 4 columns we obtained the fits

$$h_0(y) = yh_1(y) \stackrel{?}{=} \frac{y^4}{(1-y)(1-y^2)(1-y^3)}\,, \tag{23}$$

$$yh_2(y) \stackrel{?}{=} (1+y)h_1(y)\,, \tag{24}$$

$$yh_3(y) \stackrel{?}{=} (1+y^2)h_2(y)\,, \tag{25}$$

by the mere device of inserting $1/(1 - y^3)$ in the transparent fits

$$\overline{h}_0(y) = y\overline{h}_1(y) \stackrel{?}{=} \frac{y^4}{(1-y)(1-y^2)}\,, \tag{26}$$

$$y\overline{h}_2(y) \stackrel{?}{=} (1+y)\overline{h}_1(y)\,, \tag{27}$$

$$y\overline{h}_3(y) \stackrel{?}{=} (1+y^2)\overline{h}_2(y)\,. \tag{28}$$

to *all* of the results with $m \leq 20$ and $u \leq 6$ given in [4] for the contributions to (13) coming from orientable surfaces, i.e. from Lie algebras of type sl.

The challenge was then to use the posited factor $1/(1 - y - x^2)$ to marry (17–22) with (23–25). This was achieved as follows.

3 Conjecture

It is conjectured that the numbers of primitive Vassiliev invariants are generated by

$$b(x,y) := \sum_{j,k\geq 0}(\beta_{2j+k,2j}-1)x^j y^k \stackrel{?}{=} \frac{b_0 y^4 + b_1 x y^3 + b_2 x^2 y^2}{1-x^3} + \frac{b_3 x^3 y + b_4 x^4}{(1-x^3)(1-y-x^2)}\,, \tag{29}$$

with

$$b_0 = b_1 = \frac{b_2}{1+y} = \frac{b_3}{1-y^3} = 1 + b_4 = \frac{1}{(1-y)(1-y^2)(1-y^3)}\,. \tag{30}$$

This is consistent with all currently available values and bounds for $\beta_{m,u}$ and leads to

$$p(y) := \sum_{m\geq 1}(P_m - 1)y^m \stackrel{?}{=} \frac{y^4 - y^8 - y^{10} - y^{12} - y^{17}}{(1-y)(1-y^2)(1-y^3)(1-y^6)(1-y-y^4)}\,, \tag{31}$$

with $P_m := \sum_{u\geq 2}\beta_{m,u}$ enumerating primitive chord diagrams.

4 Comments and conclusions

We note the following features of (29,30) and their corollary (31).

1. It was assumed that $(1-y)(1-y^2)(1-y^3)(1-x^3)(1-y-x^2)b(x,y)$ is polynomial in x and y and that $b(\infty,y) = b(x,\infty) = 0$. This was motivated by the MZV analogies in (17–19) and by the pseudopolynomial fits of (20–25).

2. Thus Ansatz (29,30) was fully determined by the data of Table 1 with $m-6 \leq u \leq 8$. The remaining 29 data of Table 1 were successful predictions. It is remarkable that the simple pseudopolynomials of (30) fit the entirety of Table 1 and satisfy all further results and bounds. If the generator proves to be somewhat different, it will be interesting to see how it preserves the existing success, with comparable economy.

3. Summing over $u \geq 2$ we obtain the tallies

$$\begin{array}{lcl}
P_{13} &\stackrel{?}{=}& 11+16+20+18+10+3 = 78\\
P_{14} &\stackrel{?}{=}& 13+19+25+26+17+7+1 = 108\\
P_{15} &\stackrel{?}{=}& 15+23+31+35+28+15+3 = 150\\
P_{16} &\stackrel{?}{=}& 17+27+38+46+42+28+8+1 = 207\\
P_{17} &\stackrel{?}{=}& 20+31+45+60+60+46+19+3 = 284\\
P_{18} &\stackrel{?}{=}& 22+36+53+75+83+72+36+10+1 = 388\\
P_{19} &\stackrel{?}{=}& 25+41+62+93+111+107+64+25+4 = 532\\
P_{20} &\stackrel{?}{=}& 28+46+71+114+144+152+106+52+12+1 = 726
\end{array}$$

   which generate the unproven parts of the sequences in the abstract.

4. The parallel between orientable lower bounds, generated by (26,27,28) for $m \leq 20$, and the fits of (23,24,25) to Table 1, with $m \leq 14$, is quite remarkable.

5. The lower bounds of [4] are saturated at $m \leq 14$, for all u, and at $m \leq 17$, for $u = 2$ and for $u = m - 3$.

6. With $m = 15$, the fit yields values of $\beta_{m,u}$ that exceed, by unity, the lower bounds of [4] for $u = 4, 6, 8, 10$, from invariants detected by Lie algebras of type sl and osp, restricted to baguette diagrams with ladder insertions. For $u = 2$, it is known that such bounds are exceeded at all $m \geq 14$.

7. The expectations that $\beta_{19,16} = 25$, $\beta_{16,12} = 28$, $\beta_{15,10} = 28$ are the first cases where (20,21,22) require an invariant additional to the lower bounds of [4]. It would be very interesting to know what *upper* bound algorithms [3] yield in these cases.

8. The numerator of (31) is easy to characterize: the coefficients of y^m are determined by proven results for $m \leq 12$; thereafter they vanish, save at $m = 17$, where a contribution results from the final term in (16), which dominates at large y. This gives $\lim_{y\to\infty} p(y)/y = 1$, coming from the sole contribution with $m < u$, namely $\beta_{1,2} = 1$, which mimics the appearance of π^2 in the reduction of MZVs.

9. Were the predictions for P_m to be confirmed for $17 \geq m \geq 13$, those for $m \geq 18$ would appear to be rather secure, lending weight to the asymptotic prediction

$$\lim_{m\to\infty} P_m/r^m = \lim_{y\to 1/r} (1 - ry)p(y) \stackrel{?}{=} 1.06260548918755\ldots \tag{32}$$

with $r = 1.38027756909761\ldots$ solving $r^4 = r^3 + 1$. This comes from the singularity at $y = 1/r$ of the $1/(1 - y - y^4)$ term in (31), which results from setting $x = y^2$ in (29), in accordance with (16). The analogous singularity in (15) gives $\lim_{d\to\infty} D_{3d+3,d+1}/D_{3d,d} = r$.

10. The rational fit to Table 1 suggests that so-called *primitive* Vassiliev invariants, enumerated by $\beta_{m,u}$, are analogous to the elements in a search space for reducing MZVs to $\mathbf{Q}$-linear combinations of basis terms. In the case of MZVs, the basis terms enumerated by a rational generator include both irreducible MZVs, such as $\zeta(5,3) := \sum_{m>n>0} m^{-5}n^{-3}$, and their *products*, such as $\zeta(5)\zeta(3)$. If the successful phenomenology of the present enterprise be more than accidental, then there might be a further decomposition of the invariants enumerated by $\beta_{m,u}$, so far undetected in the rational domain of Vassiliev invariants, while its counterpart is readily detectable by the PSLQ algorithm [6, 35] in the irrational domain of MZVs.

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