Partial Sums of Multiple Zeta Value Series II: Finiteness of p-Divisible Sets *

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Abstract. In this paper we continue to study the partial sums of the multiple zeta value series (abbreviated as MZV series). We conjecture that for any prime p and any MZV series there is always some N such that if $n > N$ then p does not divide the numerator of the nth partial sum of the MZV series. This generalizes a conjecture of Eswarathasan and Levine and Boyd for harmonic series. We provide a lot of evidence for this general conjecture and make some heuristic argument to support it.

1 Introduction

In [13] we have studied the partial sums of the multiple zeta value series (abbreviated as MZV series) which are defined as

$$\zeta(\vec{s}\,) := \zeta(s_1, \dots, s_d) = \sum_{0<k_1<\cdots<k_d} k_1^{-s_1} \cdots k_d^{-s_d} \tag{1}$$

for $\vec{s} = (s_1, \dots, s_d) \in \mathbb{N}^d$. We call $\mathrm{wt}(\vec{s}\,) := s_1 + \cdots + s_d$ the weight and d the depth. These generalize the notion of harmonic series $\zeta(1)$ whose weight is equal to 1. The main task in [13] is to provide generalizations of Wolstenholme's Theorem for the partial sums of MZV series.

Recall that for $\vec{s} = (s_1, \dots, s_d) \in \mathbb{N}^d$ we denote the nth partial sum of MZV series by

$$H(\vec{s}; n) := \sum_{1\le k_1<\cdots<k_d\le n} k_1^{-s_1} \cdots k_d^{-s_d}, \quad n \in \mathbb{Z}_{\ge 0}. \tag{2}$$

By convention we set $H(\vec{s}; r) = 0$ for $r = 0, \dots, d-1$, and $H(\emptyset; 0) = 1$. To save space, for an ordered set $(e_1, \dots, e_t)$ we denote by $\{e_1, \dots, e_t\}^d$ the ordered set formed by repeating $(e_1, \dots, e_t)$ d times. One of the main results in [13] is the following generalization of Wolstenholme's Theorem to homogeneous MZV series

Theorem 1.1. [13, Thm. 2.13]) *Let s and d be two positive integers. Let p be an odd prime such that $p \ge d+2$ and $p-1$ divides none of sl and $sl+1$ for $l = 1, \dots, d$. Then*

$$H(\{s\}^d; p-1) \equiv \begin{cases} 0 & \pmod{p} \text{ if } sd \text{ is even,} \\ 0 & \pmod{p^2} \text{ if } sd \text{ is odd.} \end{cases}$$

In particular, the above is always true if $p \ge sd + 3$.

One can also investigate the partial sums $H(\vec{s}; n)$ with fixed $\vec{s}$ but varying n. Such a study for harmonic series was initiated systematically by Eswarathasan and Levine [7] and Boyd [2], independently. It turns out that to obtain precise information one has to study Wolstenholme type congruences in some detail and so these two directions of research are interwoven into each other rather tightly. To state our main results and conjectures we define

$$H(\vec{s}; n) = \frac{a(\vec{s}; n)}{b(\vec{s}; n)}, \quad a(\vec{s}; n),\ b(\vec{s}; n) \in \mathbb{N}, \quad \gcd(a(\vec{s}; n), b(\vec{s}; n)) = 1.$$

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For completeness, we set $a(\vec{s};0) = 0$ and $b(\vec{s};0) = 1$. Fixing a prime p we are interested in p-divisibility of the integers $a(\vec{s};n)$ and $b(\vec{s};n)$ for varying n. Thus we put $H(\vec{s};n)$ inside $\mathbb{Q}_p$, the fractional field of the p-adic integers and let v_p be the discrete valuation on $\mathbb{Q}_p$ such that $v_p(p) = 1$. In this general situation we're forced to change the notation used by the previous authors. For any $m \in \mathbb{N}$ and $\vec{s} \in \mathbb{N}^d$, put

$$I(\vec{s}|m) :=\{n \in \mathbb{Z}_{\geq 0} : b(\vec{s};n) \not\equiv 0 \pmod{m}\},$$
$$J(\vec{s}|m) :=\{n \in \mathbb{Z}_{\geq 0} : a(\vec{s};n) \equiv 0 \pmod{m}\}.$$

Note that $J(\vec{s}|m) \neq \emptyset$ since $0 \in J(\vec{s}|m)$ always. For any prime p we call $J(\vec{s}|p)$ the *p-divisible set* of (the partial sums of) the MZV series $\zeta(\vec{s})$ defined by (1).

In [2] Boyd presented a heuristic argument by modeling on simple branching processes to convince us that the p-divisible set of the harmonic series is finite for every prime p (this is also independently conjectured by Eswarathasan and Levine [7, Conjecture A]). Boyd also proves this conjecture for all primes less than 550 except for 83, 127 and 397. We now provide a generalization:

Conjecture 1.2. *Let d be a positive integer and $\vec{s} \in \mathbb{N}^d$. Then the p-divisible set $J(\vec{s}|p)$ is finite for every prime p.*

Although we are not able to prove this conjecture in general, we obtain a lot of partial results. The primary tool to prove these when $d \geq 2$ is our Criterion Theorem 2.1. Fixing an arbitrary prime p we define

$$G_0 = \{0\} \text{ and } G_t = \{n : p^{t-1} \leq n < p^t\} \text{ for } t \in \mathbb{N}.$$

Criterion Theorem Let $d \geq 2$ be a positive integer and p be a prime such that $d \in G_{t_0}$. Let $\vec{s} = (s_1, \cdots, s_d) \in \mathbb{N}^d$ and put $m = \min\{s_i : 1 \leq i \leq d\}$. For $t \in \mathbb{N}$ set $f(\vec{s}, p; t) = \min\{-v_p\big(H(\vec{s};n)\big) : n \in G_t\}$. If there is $\tau > t_0$ such that

$$f(\vec{s}, p; \tau) > (\mathrm{wt}(\vec{s}) - m)(\tau - 1) - m,$$

then $J(\vec{s}|p)$ is finite.

We list only some results obtained by applying our Criterion Theorem below. More examples including those when $d = 1$ can be found in sections 2-4 or in the online supplement [12].

Theorem 1.3. *The p-divisible set $J(\vec{s}|p)$ is finite if*

1. *$\vec{s} = (1, 1)$ and $p = 3, 7, 13, 31$, or $\vec{s} = (1, 1, 1)$ and $p = 3$, or $\vec{s} = (1, 1, 2)$ and $p = 7$.*
2. *$\vec{s} = (4, 3, 5)$ or $\vec{s} = (5, 3, 4)$ and $p = 17$.*
3. *$\vec{s} = \{s\}^d$, $1 \leq d \leq 20$, $s \geq 2$, and $p = 2$.*
4. *$\vec{s} = (s, t)$, $s, t \leq 20$, $t \geq 2$, and $p = 2, 3, 5$.*
5. *$\vec{s} = (r, s, t)$, $r, s, t \leq 10$, $t \geq 2$, and $p = 2, 3, 5$.*
6. *$\vec{s} = (q, r, s, t)$, $q, r, s, t \leq 4$, $t \geq 2$, and $p = 2, 3, 5$.*

Moreover, for $\vec{s}$ in the last four cases we have $J(\vec{s}|2) = \{0\}$.

Conjecture 1.4. *For all positive integer d and $\vec{s} \in \mathbb{N}^d$ the 2-divisible set $J(\vec{s}|2) = \{0\}$.*

In [7, Conjecture B] Eswarathasan and Levine state that there should be infinitely many primes p (so called harmonic primes) such that $J(1|p) = \{0, p-1, p^2-p, p^2-1\}$. Boyd [2] further suggest $1/e$ as the expected density of such primes. For any $\vec{s} \in \mathbb{N}^d$ we extend this notion to define the *reserved (divisibility) set* $RJ(\vec{s};x)$ of polynomials in x with rational coefficients. For any prime $p \geq \mathrm{wt}(\vec{s}) + 3$ we have $RJ(\vec{s};p) \subseteq J(\vec{s}|p)$ and there are primes p (called *reserved primes* for $\vec{s}$) such that equality holds. We determine $RJ(\vec{s})$ for many types of $\vec{s}$ in Thm. 7.2. Further we argue heuristically that the following conjecture should be true.

Conjecture 1.5. *Let $\vec{s} \in \mathbb{N}^d$. If $d = 1, \vec{s} = s \geq 2$ then the proportion of primes p with $J(\vec{s}|p) = RJ(\vec{s})$ is $1/\sqrt{e}$. This proportion is equal to $1/e$ for all other $\vec{s}$.*

This conjecture is supported by very strong numerical and theoretical evidence which we gather online [11] and in Thm. 7.2. It also generalizes Boyd's density conjecture of the harmonic primes.

At the end of this paper we put forward some more conjectures of $J(\vec{s}|p)$ related to the distribution of irregular primes.

2 A process to determine $J(\vec{s}|p)$

For any positive integer n let $n = p\tilde{n} + r$, where $\tilde{n}, r \in \mathbb{N}$ and $0 \leq r \leq p-1$. For any $\vec{s} \in \mathbb{N}^d$ define

$$H^*(\vec{s};n) = \sum_{\substack{1\leq k_1<\cdots<k_d\leq n\\ (p,k_1)=\cdots=(p,k_d)=1}} \frac{1}{k_1^{s_1}\cdots k_d^{s_d}}.$$

Then by a straightforward computation using the shuffle trick we have: for any $s, d \in \mathbb{N}$

$$H(s;n) = H^*(s;n) + p^{-s}\cdot H(s;\tilde{n}), \tag{3}$$

$$H(\{s\}^d;n) = \sum_{l=0}^{d} p^{-l}\cdot H(\{s\}^l;\tilde{n})\cdot H^*(\{s\}^{d-l};n). \tag{4}$$

where $H(\{s\}^0;m) = H^*(\{s\}^0;m) = 1$ for any integer m. We omit the proofs of these formulas whose main ingredient is contained in the proof of the main Criterion Theorem 2.1 below. Both of these formulate are generalizations of [7, (2.2)] for partial sums of harmonic series. They are the primary tools to study Conj. 1.2 for homogeneous MZV series.

For more general MZV series we need a more complicated version of these formula. Fixing an arbitrary prime p we define

$$G_0 = \{0\} \text{ and } G_t = \{n : p^{t-1} \leq n < p^t\} \text{ for } t \in \mathbb{N}.$$

For any $\vec{s} \in \mathbb{N}^d$ we set $J_t(\vec{s}|p) = G_t \cap J(\vec{s}|p)$.

Theorem 2.1. (*Criterion Theorem*) *Let $d \geq 2$ be a positive integer and p be a prime such that $d \in G_{t_0}$. Let $\vec{s} = (s_1, \cdots, s_d) \in \mathbb{N}^d$ and put $m = \min\{s_i : 1 \leq i \leq d\}$. For $t \in \mathbb{N}$ set $f(\vec{s}, p; t) = \min\{-v_p\big(H(\vec{s};n)\big) : n \in G_t\}$. If there is $\tau > t_0$ such that*

$$f(\vec{s}, p; \tau) > (\mathrm{wt}(\vec{s}) - m)(\tau - 1) - m,$$

then $J(\vec{s}|p)$ is finite.

Proof. Let $n = p\tilde{n} + r \in G_{\tau+1}$. By definition we have

$$H(\vec{s};n) = \sum_{\substack{\alpha+\beta=d\\ \alpha,\beta\geq 0}} \sum_{\substack{1\leq i_1<\cdots<i_\alpha\leq n\\ 1\leq j_1<\cdots<j_\beta\leq n\\ \{1,\dots,n\}=\{i_1,\dots,i_\alpha\}\cup\{j_1,\dots,j_\beta\}}} \sum_{\substack{K_{i_l}=pk_{i_l},1\leq l\leq\alpha\\ K_{j_l}=k_{j_l},(k_{j_l},p)=1,1\leq l\leq\beta\\ 1\leq K_1<\cdots<K_d\leq n}} \frac{1}{K_1^{s_1}\cdots K_d^{s_d}}. \tag{5}$$

Note that the terms corresponding to $\alpha = d, \beta = 0$ form the series $A = H(\vec{s};\tilde{n})/p^{\mathrm{wt}(\vec{s})} \neq 0$ since $\tau > t_0$ so that $\tilde{n} \geq p^{t_0} > d$. For all other terms with $\beta \geq 1$ we have the natural bound

$$v_p(K_1^{s_1}\cdots K_d^{s_d}) \leq (\mathrm{wt}(\vec{s}) - m)\tau$$

since $K_j < p^{\tau+1}$ for all j and one of them is prime to p. Set $B = H(\vec{s};n) - A$ then obviously $v_p(B) \geq -(\mathrm{wt}(\vec{s}) - m)\tau$. Since $\tilde{n} \in G_\tau$ by assumption of τ we know that

$$v_p(A) < -\mathrm{wt}(\vec{s}) - (\mathrm{wt}(\vec{s}) - m)(\tau-1) + m = -(\mathrm{wt}(\vec{s}) - m)\tau \leq v_p(B).$$

By induction it's easy to see that for all $t > \tau$ and $n \in G_t$ we have

$$v_p\big(H(\vec{s};n)\big) < -\mathrm{wt}(\vec{s})(t-\tau) - (\mathrm{wt}(\vec{s}) - m)(\tau-1) + m = -\mathrm{wt}(\vec{s})(t-1) + m\tau < 0.$$

This shows clearly that $J(\vec{s}|p)$ is finite. ∎

Corollary 2.2. *Let s, d be two positive integers, $d \geq 2$, and p be a prime. Suppose $d \in G_{t_0}$. Then the p-divisible set $J(\{s\}^d|p)$ is finite if there exists $\tau > t_0$ such that $f_d(\tau) > (d-1)s\tau - s$.*

Proposition 2.3. *Let r, s, t be three positive integers. Let $\vec{s} = (r, s)$ with $1 \leq r \leq 10$ and $2 \leq s \leq 10$, or $\vec{s} = (r, s, t)$ with $2 \leq r, s, t \leq 5$. Then there's always some prime $p \geq \mathrm{wt}(\vec{s}) + 3$ such that the p-divisible set $J(\vec{s}|p) = RJ(\vec{s}; p)$ is finite where $RJ(\vec{s}; p)$ is given in Thm 7.2.*

Proof. The set $RJ(\vec{s}; p)$ will be defined for general $\vec{s}$ in Definition 7.1 and computed in Thm 7.2. The proof of the proposition follows from the Criterion Theorem 2.1 by computation. To save space we put the details online [12]. □

3 Finiteness of $J(s|p)$

We now describe an approach to determine the p-divisible set $J(s|p)$ for any given positive integer s and odd prime p. This is essentially discovered by Eswarathasan and Levine [7] and by Boyd [2], independently. It follows quickly from (3) that

$$n \in I(s|p) \text{ if and only if } \tilde{n} \in J(s|p^s). \tag{6}$$

Therefore

$$n \in J(s|p) \text{ implies } \tilde{n} \in J(s|p^s). \tag{7}$$

It's also clear that

$$I(s|p) = pJ(s|p^s) + R, \quad R = \{0, 1, \cdots, p-1\}.$$

Remark 3.1. The case when $s > 1$ is very different from that of $s = 1$ considered by previous authors in that the information of $I(s|p)$ is in general not enough to determine $J(s|p)$.

To get an equivalent condition of (7) we need a partial generalization of [7, Lemma 3.1]. Set the parity function $\mathfrak{p}(m) = 1$ if m is odd and $\mathfrak{p}(m) = 2$ if m is even.

Lemma 3.2. *Let p be an odd prime, s and d be two positive integers. If $p-1 \nmid s, s+1$ then we have*

$$H^*(s; pn) \equiv 0 \pmod{p^{\mathfrak{p}(s-1)}}. \tag{8}$$

Proof. By definition

$$H^*(s; pn) = \sum_{\substack{1 \leq k \leq n \\ (p,k)=1}} \frac{1}{k^s} = \sum_{m=0}^{n-1} \left(\sum_{mp < k < (m+1)p} \frac{1}{k^s} \right). \tag{9}$$

The lemma follows from the fact that each inner sum in the parentheses satisfies the congruence in (8) which can be proved by the same argument as that in the proof of [13, Lemma 2.2] (when n is odd the shorter proof suffices). It also follows from [10, Cor. 1]. □

Proposition 3.3. *Let $s, d \in \mathbb{N}$ and p be an odd prime such that $p \geq d+2$ and $p-1$ divides none of sl and $sl+1$ for $l = 1, \ldots, d$. Then*

$$H^*(\{s\}^d; pn) \equiv 0 \pmod{p^{\mathfrak{p}(sd-1)}}.$$

The proof as well as the result itself is so similar to that of Thm. 1.1 that we leave it to the interested readers. The first step of induction is given as Lemma 3.2 above. In fact, the proposition itself reduces to Thm. 1.1 when $n = 1$.

Definition 3.4. For $n \in J(s|p^s)$ there is a unique integer $\psi_s(s|p; n) \in [0, p-1]$ such that

$$\psi_s(s|p; n) \equiv \frac{1}{p^s} H(s; n) \pmod{p}. \tag{10}$$

Lemma 3.5. *For $n = p\tilde{n} + r$, $0 \le r < p$, we have*

$$H^*(s;n) - H^*(s;p\tilde{n}) \equiv H(s;r) \pmod p. \tag{11}$$

Furthermore, if $\tilde{n} \in J(s|p^s)$ then

$$H(s;n) \equiv H(s;r) + \psi_s(s|p;\tilde{n}) \pmod p \tag{12}$$

Proof. This follows from (3) and Lemma 3.2. Also see the proof of [7, Lemma 3.2]. □

Theorem 3.6. *Let $n = p\tilde{n} + r$, $0 \le r < p$. Then $n \in J(s|p)$ if and only if*

$$\tilde{n} \in J(s|p^s) \text{ and } H(s;r) + \psi_s(\tilde{n}) \equiv 0 \pmod p. \tag{13}$$

Proof. If $n \in J(s|p)$ then (7) implies that $\tilde{n} \in J(s|p^s)$. In addition, the congruence in (13) follows immediately from (12). On the other hand, if (13) holds then (12) implies that $n \in J(s|p)$ and the proof is complete. □

We now use the above theorem to define a branching process by using the sets G_t which will compute $J(s|p)$ if it's finite.

Proposition 3.7. *Let s be a positive integer and p an odd prime. Then $J(s|p) = \cup_{t=0}^{\infty} J_t(s|p)$ where $J_t(s|p)$ can be determined recursively by*

$$J_{t+1}(s|p) = \{n = p\tilde{n} + r : \tilde{n} \in J_t(s|p^s), r \in R, v_p\big(H(s;r) + \psi_s(\tilde{n})\big) > 0\}$$

for $t \in \mathbb{N}$. Here, as before, $R = \{0, 1, \cdots, p-1\}$.

The next corollary follows naturally.

Corollary 3.8. *Let s be a positive integer and p an odd prime. Then $J(s|p)$ is finite if and only if $J_t(s|p^s) = \emptyset$ for some $t \in \mathbb{N}$.*

An easy computation according to Cor. 3.8 yields the following concrete result.

Proposition 3.9. *Let s be a positive integer. Then $J(s|p)$ is finite for primes $p = 2, 3, 5, 7$.*

Proof. (1) $p = 2$. We claim that $J(s|2) = \{0\}$. We can prove that 2 does not divide $H(s;n)$ by induction on n. This is clear for $n = 1$ and $n = 2$ because $H(s;1) = 1, H(s;2) = (1 + 2^s)/2^s$. Suppose $r \notin J(s|2)$ for all $r \le n$ and $n \in J(s|2)$. If n is odd then let $H(s;n-1) = \frac{a}{2b}$ where a is odd by inductive assumption. Then

$$H(s;n) = \frac{a}{2b} + \frac{1}{n^s} = \frac{Na + 2B}{\text{l.c.m}(2b, n^s)},$$

where $N = n^s/\gcd(n^s, b)$ and $B = b/\gcd(n^s, b)$. Hence $Na + 2B$ is odd because both N and a are odd, which is a contradiction. If $n = 2\tilde{n}$ then

$$H(s;2\tilde{n}) = \sum_{k=1}^{\tilde{n}} \left(\frac{1}{(2k-1)^s} + \frac{1}{(2k)^s} \right) \equiv \tilde{n} + \frac{1}{2^s} H(s;\tilde{n}) \pmod 2.$$

By inductive assumption $2 \nmid H(s;\tilde{n})$ which implies that $2 \nmid H(s;2\tilde{n})$. So n can not belong to $J(s|2)$ either if n is even. This shows that $J(s|2) = \{0\}$. In fact, it is not hard to see that for $n \in G_t$, $t \ge 1$ we have

$$v_2\big(H(s;n)\big) = -(t-1)s. \tag{14}$$

For $3 \le p \le 7$ Eswarathasan and Levine [7] have shown that $J(1|p)$ are finite. We also know that when $s \le 4$ then $J(s|p)$ are finite for these primes by explicit computation [12]. Assume $s \ge 4$. Then by Cor. 3.8 we only need to show that $J_1(s|p^s) = \emptyset$. We need [13, Cor. 2.7] which implies that if $p \ge 3$ is a regular prime then

$$H(s;p-1) \not\equiv 0 \pmod{p^s} \text{ for } s \ge 4. \tag{15}$$

(2) $p = 3$. Neither $H(s;1) = 1$ nor $H(s;2) = 1 + 1/2^s$ is divisible by 3^s. so $J_1(s|3^s) = \emptyset$.
(3) $p = 5$. Neither $H(s;1) = 1$ nor $H(s;2) = 1 + 1/2^s$ is divisible by 5^s. Now

$$6^s H(s;3) = 2^s + 3^s + 6^s \equiv 2^s + (-2)^s + 1 \equiv \begin{cases} 2 \cdot 4^n + 1 & \pmod 5 \quad \text{if } s = 2n, \\ 1 & \pmod 5 \quad \text{if } s \text{ is odd.} \end{cases}$$

So we always have $H(s;3) \not\equiv 0 \pmod 5$, i.e., $3 \notin J_1(s|5^s)$. Finally, (15) implies that $4 \notin J_1(s|5^s)$ for $s \geq 4$ because 5 is a regular prime. Hence $J_1(s|5^s) = \emptyset$.

(4) $p = 7$. Clearly $1, 2 \notin J_1(s|7^s)$ and $6^s H(s;3) = 2^s + 3^s + 6^s < 7^s$ when $s \geq 4$. Now

$$H(s;4) = H(s;6) - \frac{1}{5^s} - \frac{1}{6^s} \equiv (-1)^{s+1} \left(1 + \frac{1}{2^s}\right) \pmod 7.$$

Because $2^3 \equiv 1 \pmod 7$ we get

$$1 + \frac{1}{2^s} \equiv \begin{cases} 2 & \pmod 7 \quad \text{if } s \equiv 0 \pmod 3, \\ 3/2 & \pmod 7 \quad \text{if } s \equiv 1 \pmod 3, \\ 3 & \pmod 7 \quad \text{if } s \equiv -1 \pmod 3. \end{cases}$$

Therefore $4 \notin J_1(s|7^s)$. Similarly, $H(s;5) \equiv (-1)^{s+1} \not\equiv 0 \pmod 7$. Finally, it follows from (15) that $6 \notin J_1(s|7^s)$ for $s \geq 4$. These show that $J_1(s|7^s) = \emptyset$ for all $s \geq 4$. □

Remark 3.10. The case $p = 11$ is not so easy since $H(3;4) \equiv 0 \pmod{11}$ and moreover, for any positive integer e there is some $s < p^e(p-1)$ such that $H(s;4) \equiv 0 \pmod{11^{e+1}}$.

We also computed $J(s|p)$ for some other s and p (see [12]), which confirms the following

Proposition 3.11. *Let p be a prime such that $p \leq 3001$. Then $J(s|p)$ is finite for $2 \leq s \leq 300$.*

4 Finiteness of $J(\{s\}^d|p)$

In order to apply Criterion Theorem 2.1 we set

$$f_d(t) := f(\{s\}^d, p; t) = \min\{-v_p(H(\{s\}^d; n)) : n \in G_t\}, \quad \forall t \geq 1.$$

We first look at the case $s \geq 2$.

Lemma 4.1. *For all $s \geq 2$ we have $v_2(3^s + 1) = \mathfrak{p}(s-1)$ which is 1 if s is even and 2 if s is odd. In particular, we always have $3^s + 1 \not\equiv 0 \pmod{2^s}$.*

Proof. This is clear because

$$3^s + 1 = \begin{cases} 9^n + 1 \equiv 2 & \pmod 8 \quad \text{if } s = 2n, \\ 3 \cdot 9^n + 1 \equiv 4 & \pmod 8 \quad \text{if } s = 2n+1. \end{cases}$$

□

Proposition 4.2. *Let $s \geq 2$ and $d \leq 20$ be two positive integers. Then the 2-divisible set $J(\{s\}^d|2)$ is finite.*

Proof. When $d = 1$ this is included in Prop. 3.9. So we assume $s, d \geq 2$. Then

$$H(s;2) = 1 + \frac{1}{2^s}, \quad H(s,s;2) = \frac{1}{2^s}, \quad H(s;3) = \frac{6^s + 3^s + 2^s}{6^s}.$$

Further, by Lemma 4.1 we know that

$$H(s,s;3) = \frac{1}{2^s} + \left(1 + \frac{1}{2^s}\right)\frac{1}{3^s} = \frac{3^s + 1 + 2^s}{6^s}$$

has at least a factor 2 in the denominator. Therefore we can take $\tau = 2$ to get $f(\tau) \geq 1 > (2s-s)(\tau-1)-s = 0$. So the condition in Cor. 2.2 is satisfied and consequently $J(s,s|2) = \{0\}$.

A detailed study of using Lemma 4.1 tells more. Let $t \geq 0$ and $n \in G_{t+2}$. Then by induction and equation (4) we can easily show that

$$v_2\big(H(s,s;n)\big) = \begin{cases} -(2t+1)s & \text{if } 2^{t+1} \leq n < 2^{t+1}+2^t, \\ \mathfrak{p}(s-1)-(2t+1)s & \text{if } 2^{t+1}+2^t \leq n < 2^{t+2}. \end{cases} \tag{16}$$

Putting $d = 3$ in the following equation

$$H(\{s\}^d;n) = H(\{s\}^d;n-1) + \frac{1}{n^s} H(\{s\}^{d-1};n-1), \tag{17}$$

and applying induction on t we can show that

$$v_2\big(H(s,s,s;n)\big) = \begin{cases} \mathfrak{p}(s-1)-3ts & \text{if } 2^{t+1} \leq n < 2^{t+1}+2^{t-1}, \\ -3ts & \text{if } 2^{t+1}+2^{t-1} \leq n < 2^{t+1}+2^t, \\ -(3t+1)s & \text{if } 2^{t+1}+2^t \leq n < 2^{t+2}. \end{cases} \tag{18}$$

So we get $J(s,s,s|2) = \{0\}$ when $s \geq 2$.

When $d \geq 4$ we can utilize (17) again. However, even in the case $d = 4$ it is very complicated already. Nevertheless the idea is straightforward so we omit the details of the proof. Suppose $s = 2$ and $n \in G_{t+2}$ with $t \geq 1$ (note that $H(\{s\}^4;n) = 0$ for all $n \leq 3$). Then we have

$$v_2\big(H(\{2\}^4;n)\big) = \begin{cases} (1) \quad -2(4t-1) & \text{if } 2^{t+1} \leq n < 2^{t+1}+2^t, \\ (2) \quad -8t & \text{if } 2^{t+1}+2^t \leq n < 2^{t+1}+2^t+2^{t-1}, \\ (3) \quad -8t+\delta(t) & \text{if } 2^{t+1}+2^t+2^{t-1} \leq n < 2^{t+1}+2^t+2^{t-1}+2^{t-4}, \\ (4) \quad -8t+7 & \text{if } 2^{t+1}+2^t+2^{t-1}+2^{t-4} \leq n < 2^{t+1}+2^t+2^{t-1}+2^{t-3}, \\ (5) \quad -2(4t-2) & \text{if } 2^{t+1}+2^t+2^{t-1}+2^{t-3} \leq n < 2^{t+1}+2^t+2^{t-1}+2^{t-2}, \\ (6) \quad -2(4t-1) & \text{if } 2^{t+1}+2^t+2^{t-1}+2^{t-2} \leq n < 2^{t+2}. \end{cases} \tag{19}$$

Here if $t = 1$ then (3)-(6) merge into (6); if $t = 2$ then $\delta(t) = 5$ and (3)-(5) merge into (3); if $t = 3$ then (3) and (4) merge into (3); if $t \geq 3$ then $\delta(t) = 6$. When $s = 3$ and $n \in G_{t+2}$ with $t \geq 1$ we have

$$v_2\big(H(\{3\}^4;n)\big) = \begin{cases} (1) \quad -3(4t-1) & \text{if } 2^{t+1} \leq n < 2^{t+1}+2^t, \\ (2) \quad -12t & \text{if } 2^{t+1}+2^t \leq n < 2^{t+1}+2^t+2^{t-1}, \\ (3) \quad -3(4t-1) & \text{if } 2^{t+1}+2^t+2^{t-1} \leq n < 2^{t+1}+2^t+2^{t-1}+2^{t-2}, \\ (4) \quad -3(4t-1)+1 & \text{if } 2^{t+1}+2^t+2^{t-1}+2^{t-2} \leq n < 2^{t+2}. \end{cases} \tag{20}$$

Here if $t = 1$ then (3) and (4) merge into (4). When $s \geq 4$ we have

$$v_2\big(H(\{s\}^4;n)\big) = \begin{cases} (1) \quad -s(4t-1) & \text{if } 2^{t+1} \leq n < 2^{t+1}+2^t, \\ (2) \quad -4st & \text{if } 2^{t+1}+2^t \leq n < 2^{t+1}+2^t+2^{t-1}, \\ (3) \quad -4st+2\,\mathfrak{p}(s-1) & \text{if } 2^{t+1}+2^t+2^{t-1} \leq n < 2^{t+2}. \end{cases} \tag{21}$$

Equations (19)-(21) imply that $J(\{s\}^4|2) = \{0\}$ for all $s \geq 2$.

Similar computation shows that when $d = 5$ and $n \in G_{t+2}$ with $t \geq 1$ we have

$$v_2\big(H(\{2\}^5;n)\big) = \begin{cases} (1) \quad -s(5t-3)+2\,\mathfrak{p}(s-1) & \text{if } 2^{t+1} \leq n < 2^{t+1}+2^{t-3}, \\ (2) \quad -s(5t-3)+3 & \text{if } 2^{t+1}+2^{t-3} \leq n < 2^{t+1}+2^{t-2}, \\ (3) \quad -s(5t-3) & \text{if } 2^{t+1}+2^{t-2} \leq n < 2^{t+1}+2^{t-1}, \\ (4) \quad -s(5t-2) & \text{if } 2^{t+1}+2^{t-1} \leq n < 2^{t+1}+2^t, \\ (5) \quad -s(5t-1) & \text{if } 2^{t+1}+2^t \leq n < 2^{t+1}+2^t+2^{t-1}, \\ (6) \quad -s(5t-1)+1 & \text{if } 2^{t+1}+2^t+2^{t-1} \leq n < 2^{t+2}. \end{cases} \tag{22}$$

Here if $t = 1$ then (1)-(3) do not appear; if $s \geq 3$ then (1) and (2)) merge into (1). This implies that $J(\{s\}^5|2) = \{0\}$ for all $s \geq 2$.

As d gets larger there are more and more cases. The number of cases, denoted by $C(d)$, is independent of s when s is large enough and tends to increase with d though not always. We compute the following

$$C(6) = 5, \quad C(7) = 7, \quad C(8) = 6, \quad C(9) = 8, \quad C(10) = 8, \quad C(11) = 11, \ C(12) = 10,$$
$$C(13) = 12, \ C(15) = 15, \ C(16) = 12, \ C(17) = 15, \ C(18) = 14, \ C(19) = 18, \ C(20) = 15.$$

After tedious verification we find $J(\{s\}^d|2) = \{0\}$ for all $d \leq 20$ and $s \geq 2$. □

For any given d by similar method we should be able to determine $J(\{s\}^d|2)$ for all $s \geq 2$. However, for odd primes we can only extend this to small d and small s by computer computation.

Proposition 4.3. *Let s and d be two positive integers. Suppose $2 \leq s \leq 10$ and $2 \leq d \leq 10$. Then the p-divisible set $J(\{s\}^d|p)$ is finite for the consecutive five primes immediately after $sd + 2$. Moreover there's always some prime p such that $J(\{s\}^d|p) = RJ(\{s\}^d;p)$ where*

$$RJ(\{s\}^d;p) = \begin{cases} \{0, p-1\} & \text{if } 2 \nmid s, \\ \{0, i + (p-1)/2, p-1 : 0 \leq i \leq d-1\} & \text{if } 2|s. \end{cases}$$

Proof. The set $RJ(\vec{s};p)$ will be defined for general $\vec{s}$ in Definition 7.1 and computed in Thm 7.2. The proof of the proposition follows from Cor. 2.2 by computer computation. To save space we put the details online [12]. □

In the rest of this section we turn to the case $s = 1$. We may assume $d \geq 2$ since the harmonic series has been handled by [7] and [2]. According Cor. 2.2 if we can find τ large enough such that $f_d(\tau) \geq (d-1)(\tau - 1)$ then $J(\{1\}^d|p)$ is finite.

Proposition 4.4. *1. The p-divisible set $J(\{1\}^2|p)$ is finite if $p = 3, 7, 13, 31$.*

2. Let $s, t \leq 20$ and $t \geq 2$. Then the set $J(s, t|p)$ is finite for $p = 2, 3, 5$.

3. Let $r, s, t \leq 10$ and $t \geq 2$. Then the set $J(r, s, t|p)$ is finite for $p = 2, 3, 5$.

4. Let $q, r, s, t \leq 4$ and $t \geq 2$. Then the set $J(q, r, s, t|p)$ is finite for $p = 2, 3, 5$.

Proof. We only need to find τ satisfying the condition of Cor. 2.2.

(1) For each τ in the following we have $f_2(\tau) = \tau - 1$.

$p = 3$. Take $\tau = 6$. Then computation reveals that $J(1, 1|3) = \{0, 5\}$. If $d = 3$ then we take $\tau = 10$. Then we have $f_3(\tau) \geq 2(\tau - 1)$. Note that in G_9 there is $n = 17770$ such that $v_3\big(H(\{1\}^3;n)\big) = -15$ so $f_3(9) = 15$. By Cor. 2.2 and simple computation we see that $J(\{1\}^3|3) = \{0, 8\}$.

$p = 7$. Take $\tau = 4$. Then $J(1, 1|7) = \{0, 4, 6, 7, 13\}$.

$p = 13$. Take $\tau = 4$. Then $J(1, 1|13) = \{0, 12, 13, 25\}$.

$p = 31$. Take $\tau = 4$. Then $J(1, 1|31) = \{0, 17, 22, 30, 31, 61\}$.

For the last three cases with $p = 2, 3, 5$ we put the result of computation online [12]. For example, we can take $\tau = 10$ and show that $J(1, 1, 1|3) = \{0, 8\}$. □

Remark 4.5. We could extend our results to larger d and some other primes p but it'd be very time consuming with our slow PCs. However, even in the case $\vec{s} = (1, 1)$ similar process fails for $p = 2$. Computations suggest that $J(1, 1|2) = \{0\}$, $J(1, 1|5) = \{0, 4, 5, 9\}$, $J(1, 1|11) = \{0, 10, 11, 21\}$ and $J(1, 1|17) = \{0, 11, 13, 16, 17, 33\}$. We will analyze the situation for $p = 2$ in detail in the next section.

5 Sequences related to $J(s, 1|2)$

One may wonder what goes wrong in Proposition 4.4 if we let $\vec{s} = (1, 1)$ and $p = 2$. We will see that, amazingly, this problem might be related to some pseudo-random process.

Only in this section we adopt the shorthand $H_1(n) := H(1; n)$ and $H_2(n) := H(1, 1; n)$. Let's start with the first few partial sums of $H_2(n)$ when $2 \le n \le 14$. Here $\sim$ means we only consider the fractional part of the numbers.

$$H_2(2) \sim \frac{1}{2}, \quad H_2(3) \sim 1, \quad H_2(4) \sim \frac{11}{24}, \quad H_2(5) \sim \frac{7}{8}, \quad H_2(6) \sim \frac{23}{90},$$
$$H_2(7) \sim \frac{109}{180}, \quad H_2(8) \sim \frac{9371}{10080}, \quad H_2(9) \sim \frac{467}{2016}, \quad H_2(10) \sim \frac{25933}{50400},$$
$$H_2(11) \sim \frac{25933}{50400}, \quad H_2(12) \sim \frac{39353}{50400}, \quad H_2(13) \sim \frac{13501}{415800}, \quad H_2(14) \sim \frac{4027}{14850}.$$

It looks like 2 never divides the numerator and moreover, the 2-powers in the denominators of $H_2(n)$ tend to increase with n, though not always. To proceed we need to know the 2-divisibility of $H_1^*(n)$.

Lemma 5.1. *Let n be a positive integer. Then*

$$H_1^*(n) \equiv \begin{cases} 0 \pmod 4 & \text{if } n \equiv 0, 3 \pmod 4, \\ 1 \pmod 4 & \text{if } n \equiv 1, 2 \pmod 4. \end{cases}$$

Proof. If n is even then obviously $H_1^*(n) = H_1^*(n-1)$. So we only need to consider $n \equiv 1, 3 \pmod 4$.

Set $\delta = 1$ if $n = 4l + 1$ and $\delta = 0$ if $n = 4l - 1$. Then

$$H_1^*(n) = \frac{\delta}{4l+1} + \sum_{i=1}^{2l} \frac{1}{2i-1} = \frac{\delta}{4l+1} + \sum_{i=1}^{l} \left(\frac{1}{2i-1} + \frac{1}{4l-2i+1} \right) \equiv \delta \pmod 4$$

as desired. □

Remark 5.2. By working more carefully we can obtain the following improvement of Lemma 5.1: if $n = 2^d m$ or $n = 2^d m - 1$ where m is odd and $d \ge 1$. Then $v_2\big(H_1^*(n)\big) = 2(d-1)$. However, the proof is complicated and it is not needed in the rest of the paper so we leave the proof of this general statement to the interested readers.

The following result is exactly the reason why Cor 2.2 cannot be applied to $J(1, 1|2)$.

Proposition 5.3. *For any $t \ge 2$, there is a unique $n_t \in G_t$ such that $v_2\big(H_2(n_t)\big) \ge 2 - t$ whereas for all $n_t \ne n \in G_t$ we have $v_2\big(H_2(n)\big) \le 1 - t$. Therefore, for all positive integers $n \notin \{n_t\}_{t \ge 1}$ the numerator of $H_2(n)$ is not divisible by 2.*

Proof. Note that $G_1 = \{1\}$ and $G_2 = \{2, 3\}$. Thus $n_2 = 3$ because $H_2(3) = 1$. Assume that $t \ge 3$ and each n_i has been found in G_i uniquely for $i \le t$. Let $n = 2\tilde{n} + r \in G_{t+1}$ for $r = 0$ or 1. When $d = p = 2$ and $s = 1$ equation (4) becomes

$$H_2(n) = H_2^*(n) + \frac{1}{2} H_1(\tilde{n}) H_1^*(n) + \frac{1}{4} H_2(\tilde{n}). \tag{23}$$

It's easy to show that $v_2\big(H_1(m)\big) = 1 - t$ for $m \in G_t$ by induction and the recursive relation $H_1(n) = H_1^*(n) + H_1(\tilde{n})/2$. If $\tilde{n} \ne n_t$ then we have $v_2\big(H_2(\tilde{n})\big) \le 1 - t$ and hence

$$v_2\big(H_2(n)\big) = \min\{v_2\big(H_1^*(n)\big) - t, -1 - t\} = -1 - t < 1 - (t + 1).$$

Suppose now $\tilde{n} = n_t$ and $n = 2n_t + r_t$. We consider four possible cases.

(i) If $v_2\big(H_2(n_t)\big) = 2 - t$ and $v_2\big(H_1^*(n)\big) \ge 1$ then $n \ne n_{t+1}$ because

$$v_2\big(H_2(n)\big) = \min\{v_2\big(H_1^*(n)\big) - t, -t\} = -t = 1 - (t + 1).$$

(ii) If $v_2\big(H_2(n_t)\big)=2-t$ and $v_2\big(H_1^*(n)\big)=0$ then

$$v_2\left(\frac{1}{2}H_1(n_t)H_1^*(n)\right)=v_2\left(\frac{1}{4}H_2(n_t)\right)=-t.$$

Hence $n=n_{t+1}$ because

$$v_2\big(H_2(n)\big)\geq 1-t=2-(t+1).$$

(iii) If $v_2\big(H_2(n_t)\big)\geq 3-t$ and $v_2\big(H_1^*(n)\big)=0$ then $n\neq n_{t+1}$ because $v_2\big(H_2(n)\big)=\min\{v_2\big(H_1^*(n)\big)-t, v_2\big(H_2(n_t)\big)-2-t\}=-t=1-(t+1)$.

(iv) If $v_2\big(H_2(n_t)\big)\geq 3-t$ and $v_2\big(H_1^*(n)\big)\geq 1$ then $n=n_{t+1}$ because

$$v_2\big(H_2(n)\big)\geq\min\{v_2\big(H_1^*(n)\big)-t, v_2\big(H_2(n_t)\big)-2-t\}\geq 1-t=2-(t+1).$$

Now if $n_t=2l$ is even then by Lemma 5.1

(1) $2n_t+1\equiv 1 \pmod 4$ and $v_2\big(H_1^*(2n_t+1)\big)=0$, and

(2) $2n_t\equiv 0 \pmod 4$ and $v_2\big(H_1^*(2n_t+1)\big)\geq 1$.

If $n_t=2l+1$ is odd then by Lemma 5.1

(3) $2n_t+1\equiv 3 \pmod 4$ and $v_2\big(H_1^*(2n_t+1)\big)\geq 1$ and

(4) $2n_t\equiv 2 \pmod 4$ and $v_2\big(H_1^*(2n_t+1)\big)=0$.

Therefore, we have four situations to consider:

(a) n_t is even and $v_2\big(H_2(n_t)\big)=2-t$. Then $n_{t+1}=2n_t+1$ by (1) and (ii).

(b) n_t is even and $v_2\big(H_2(n_t)\big)\geq 3-t$. Then $n_{t+1}=2n_t$ by (2) and (iv).

(c) n_t is odd and $v_2\big(H_2(n_t)\big)\geq 3-t$. Then $n_{t+1}=2n_t+1$ by (3) and (iv).

(d) n_t is odd and $v_2\big(H_2(n_t)\big)=2-t$. Then $n_{t+1}=2n_t$ by (4) and (ii).

It follows that $n_{t+1}\in G_{t+1}$ is uniquely determined. This finishes the proof of the proposition. □

Denote the dyadic valuation $v_2\big(H_2(n_t)\big)$ by $-w_t$. Then we have the following two interesting sequences:

$$\begin{aligned}\{n_t\}_{t\geq 2}=\{&3,6,13,27,54,109,219,439,879,1759,3518,7037,14075,28151,\\&56303,112606,225212,450424,900848,1801696,3603393,\dots\}\end{aligned}\tag{24}$$

$$\{w_t\}_{t\geq 2}=\{0,1,3,4,3,3,5,7,9,10,9,10,12,14,13,13,15,17,19,19,\dots\}\tag{25}$$

Set $r_1=r_2=1$ and define $r_t=0$ or 1 for $t\geq 3$ as determined in the proof of Prop. 5.3 such that $n_{t+1}=2n_t+r_t$. Then clearly n_t can be written as

$$n_t=(r_1r_2\dots r_t)_2\tag{26}$$

in binary system and apparently the sequence $\{n_t\}$ increases very fast. Further, the occurrence of $r_t=0$ or $r_t=1$ does not seem to have any predictable pattern so we think this might be related to some pseudo-random process. By this we mean the following. First we of course conjecture that $\{w_t\}_{t\geq 3}$ is always bounded below by 1 which is equivalent to say $J(1,1|2)=\{0\}$. We also have proved that w_t is bounded above by $1-t$ and it is not hard to see that $w_t=t-1$ for infinitely many t's. It's also conceivable that w_t are near $t-1$ most of the time. However, we believe w_t could move very far away from $t-1$ for very large t. At the present stage, we could not even determine whether the difference between w_t and $t-1$ can be arbitrarily large.

Remark 5.4. We put the two sequences $\{n_t\}_{t\geq 2}$ and $\{w_t\}_{t\geq 2}$ in Sloane's online database of integer sequences as $A079403(n)$ and $A079404(n)$, respectively. Shortly after Benoit Cloitre emailed me a formula for the known terms of $\{n_t\}_{t\geq 2}$:

$$n_t=\lfloor 2^{t-1}c\rfloor\tag{27}$$

where $c=1.718232...$. Indeed, it's easy to see that

$$n_1=1, n_t=2^{t-1}\prod_{k=1}^{t-1}\left(1+\frac{r_k}{2n_k}\right),\ \forall t\geq 2.$$

Further,

$$c = \lim_{t\to\infty} \prod_{k=1}^{t-1} \left(1 + \frac{r_k}{2n_k}\right)$$

exists by comparison test. From equation (26) we get

$$c = (r_1.r_2r_3r_4\dots)_2 = (1.1011011111011110000001...)_2 = 1.718232...$$

Moreover, using binary system we see that the integral part of $2^{t-1}c$ is exactly n_t, as desired.

We can easily generalize Prop. 5.3 to the following.

Proposition 5.5. *For any $t \ge 2$, there is a unique $n_t \in G_t$ such that $v_2\big(H(s,1;n_t)\big) \ge -s(t-1)+1$ whereas for all $n_t \ne n \in G_t$ we have $v_2\big(H(s,1;n)\big) \le -s(t-1)$. Therefore, for all positive integers $n \notin \{n_t\}_{t\ge1}$ the numerator of $H(s,1;n)$ is not divisible by 2.*

Proof. We can assume that $s \ge 2$ because of Prop. 5.3. The key to the proof is equation (5) which yields that

$$H(s,1;n) = H^*(s,1;n) + U(s,1;n) + V(s,1;n) + \frac{1}{2^{s+1}} H(s,1;\tilde{n})$$

where

$$U(s,1;n) = \frac{1}{2^s} \sum_{1\le 2k<l\le n, 2\nmid l} \frac{1}{k^s l}, \quad V(s,1;n) = \frac{1}{2} \sum_{1\le k<pl\le n, 2\nmid k} \frac{1}{k^s l}.$$

Now it's easy to see that if $v_2\big(H(s,1;\tilde{n})\big) \le -s(t-1)$ then $v_2\big(H(s,1;n)\big) \le -st$.

When $t=2$ we find $n_2 = 2$ always because

$$H(s,1;2) = \frac{1}{2}, \quad H(s,1;3) = \frac{1}{2} + \frac{2^s+1}{3\cdot 2^s}.$$

Assume that $t \ge 3$ and $\tilde{n}$ is the unique $n_t \in G_t$ such that $v_2\big(H(s,1;\tilde{n})\big) > -s(t-1)$. Then $v_2\big(H(s;\tilde{n})\big) = -s(t-1)$ by equation (14). So we can always uniquely choose r_t so that for $n = 2\tilde{n} + r_t \in G_{t+1}$

$$v_2\big(U(s,1;n)\big) = v_2\big(U(s,1;2\tilde{n}) + rH(s;\tilde{n})/2^s\big) = -st$$

if $v_2\big(H(s,1;\tilde{n})\big) = -s(t-1)+1$. If $v_2\big(H(s,1;\tilde{n})\big) > -s(t-1)+1$ then we can uniquely choose r_t so that

$$v_2\big(U(s,1;n)\big) \ge -st+1.$$

The upshot is for $n_t \in G_t$ there is a unique $n_{t+1} \in G_{t+1}$ satisfying the condition of the proposition. This finishes the proof. ∎

In general, we cannot apply Criterion Theorem to determine the finiteness of $J(\vec{s}\,', 1|2)$ for any $\vec{s}\,' \in \mathbb{N}^d$, because of the existence of similar sequences. Moreover we believe 2 never divides the numerator of any partial sums of MZV series.

Conjecture 5.6. *For all positive integer d and $\vec{s} \in \mathbb{N}^d$ the 2-divisible set $J(\vec{s}|2) = \{0\}$.*

We have verified this conjecture for all $\vec{s} = (s,t)$ and $\vec{s} = (r,s,t)$ with $1 \le r,s \le 10$ and $2 \le t \le 10$, and for all $\vec{s} = (r,s,t,u)$ with $1 \le r,s,t \le 4$ and $2 \le u \le 4$. See [12]. The computation is very time-consuming, for example when $\vec{s} = (1,4,4,2)$ the Maple program runs more than 3.5 hours on my PC with Pentium 4 CPU 3.06GHZ and 512 MB RAM. The same program in GP Pari runs a little faster. We put the program at the end of our online supplement [12].

We believe that $\vec{s} = (\vec{s},1)$ are the only cases that our Criterion Theorem fails (see [12]) among all possible $\vec{s}$ and prime p. Let me sketch a heuristic argument for this belief for the case $\vec{s} = \{1\}^d$ and $p \ge 3$.

By the recursive relation

$$H(\{1\}^d;n) = \sum_{l=0}^{d} p^{-l} \cdot H(\{1\}^l;\tilde{n}) \cdot H^*(\{1\}^{d-l};n).$$

it is not hard to see that the size of τ we are looking for in the Criterion Theorem depends on the length of the sequences $\{n_t\}_{t>t_0}$ not satisfying the condition in the theorem, where $n_t \in G_t$ and $n_{t+1} = pn_t + r_t$ for some $0 \le r_t < p$. If n_t is already found then the existence of n_{t+1} depends on $H^*(1;n)$ essentially, which we assume to distribute among $(p+1)/2$ values modulo p by the symmetric structure of $J_1(1|p)$ (see section 6). So n_t produces two possible n_{t+1} or no n_{t+1} with the same probability $q = (p-1)/2p$, and it produces exactly one n_{t+1} with probability $1/p$.

Let's assume that a certain cell reproduces itself according a similar law as above, namely, it clones itself or dies in the next generation with the same probability q, and it stays alive without reproduction with probability $1/p$. Let p_k be the probability that starting from k cells in the beginning the cells eventually all die out. We claim that $p_k = 1$ for all k. Indeed, it is not too hard to see that we only need to show $p_1 = 1$. This follows from the criticality theorem for Galton-Watson branching process (see [8, Preface] or [1, p. 7, Thm. 1]) because the average offspring is $2q + 1/p = 1$.

6 The structure of $J_1(\{s\}^d|p)$

Set $J_t^0(\vec{s}|m) = \{0\} \cup J_t(\vec{s}|m)$ for any positive integers t, m and $\vec{s} \in \mathbb{N}^d$. The next result is easy but very useful in determining the structure of $J_1(s|p)$ since it tells us essentially that $J_1^0(s|p)$ is symmetric about $(p-1)/2$.

Proposition 6.1. *Let p be an odd prime and $s \in \mathbb{N}$. Let $r \in \{1, \dots, p-2\}$. Then $r \in J_1(s|p)$ if and only if $p-1-r \in J_1(s|p)$.*

Proof. If $p-1|s$ then $J_1(s|p) = \emptyset$ because $H(s;r) \equiv r \pmod p$ for all $r \in \{1, \dots, p-2\}$. If $p-1 \nmid s$ then we have

$$H(s;r) = \sum_{k=1}^{r} \frac{1}{k^s} = \sum_{k=p-r}^{p-1} \frac{1}{(p-k)^s} \equiv (-1)^s \sum_{k=p-r}^{p-1} \frac{1}{k^s} \pmod p.$$

Subtracting $0 \equiv (-1)^s \sum_{k=1}^{p-1} \frac{1}{k^s} \pmod p$ from the above we get the desired result. □

Remark 6.2. We feel prompted to mention that the symmetry of $J_1^0(s|p)$ is not enjoyed by $J_1^0(s|p^2)$. For instance, while $J_1^0(5|37) = \{0, 6, 9, 12, 18, 24, 27, 30, 36\}$ is symmetric about 18 the set $J_1^0(5|37^2) = \{0, 6, 36\}$ is not.

Now that we know $J_1^0(s|p)$ is symmetric we may wonder what happens to the center $(p-1)/2$. When s is odd the answer is related to the irregularity of primes.

Proposition 6.3. *Let p be an odd prime and s be a positive integer such that $p-1 \nmid s-1$ and $p-1 \nmid s$. If s is even then $(p-1)/2 \in J_1(s|p)$. When s is odd we let n be the unique positive integer such that $s \equiv n \pmod{p-1}$ and $2 \le n \le p-2$. Then we have*

$$H(s;(p-1)/2) \equiv \frac{2-2^n}{n} B_{p-n} \pmod{p^2}. \tag{28}$$

Therefore,

(a) If $(p, p-n)$ is an irregular pair then $(p-1)/2 \in J_1(s|p)$.

(b) If $(p-1)/2 \in J_1(s|p)$ and $2^s \not\equiv 2 \pmod p$ then $(p, p-n)$ is an irregular pair.

In particular, if $s \ge 3$ is odd and $p > 2^s - 2$ then $(p-1)/2 \in J_1(s|p)$ if and only if $(p, p-s)$ is an irregular pair.

Proof. Let p, s, and n be as given in the proposition. By Voronoi congruence for $m > 1$ we get (taking $a = 2$ and $n = p^2$ in [9, Prop. 15.2.3])

$$(2^m - 1)B_m \equiv m2^{m-1} \sum_{k=(p^2+1)/2}^{p^2-1} k^{m-1} \pmod{p^2}.$$

Replacing k by $p^2 - k$ we see that

$$(2^m - 1)B_m \equiv m(-2)^{m-1} \sum_{k=1}^{(p^2-1)/2} k^{m-1} \pmod{p^2}. \tag{29}$$

Now we break the sum into two parts: $1 \le k < p(p-1)/2$ and $p(p-1)/2 \le k \le (p^2-1)/2$. For $k < p(p-1)/2$ we write $k = pq + r$, $0 \le q \le (p-3)/2$, $0 \le r \le p-1$. Then

$$\begin{aligned}\sum_{1\le k<p(p-1)/2} k^{m-1} &= \sum_{q=0}^{(p-3)/2}\sum_{r=0}^{p-1}(pq+r)^{m-1}\\ &\equiv \sum_{q=0}^{(p-3)/2}\sum_{r=0}^{p-1}(m-1)pqr^{m-2}+r^{m-1} \equiv 0 \pmod{p^{\mathfrak{p}(m)}} \qquad (30)\end{aligned}$$

by Thm. 1.1, where $\mathfrak{p}(m) = 1, 2$ is the parity of m. For $p(p-1)/2 \le k \le (p^2-1)/2$ we write $k = p(p-1)/2 + r$ where $0 \le r \le (p-1)/2$. Then

$$\sum_{k=p(p-1)/2}^{(p^2-1)/2} k^{m-1} = \sum_{r=0}^{(p-1)/2}\left(\binom{p}{2}+r\right)^{m-1} \equiv \sum_{r=0}^{(p-1)/2}(m-1)\binom{p}{2}r^{m-2}+r^{m-1} \pmod{p^2}. \qquad (31)$$

Putting the three congruences (29), (30) and (31) together and taking $m = p - n > 1$ we obtain

$$(2^m-1)B_{p-n} \equiv m(-2)^{m-1}\left[(m-1)\binom{p}{2}H(n+1;(p-1)/2)+H(n;(p-1)/2)\right] \pmod{p^{\mathfrak{p}(m)}}. \qquad (32)$$

If s is even then $m = p - n$ is odd and $B_{p-n} = 0$ since $n \ne p-1$. Consequently

$$H(n;(p-1)/2) \equiv 0 \pmod p$$

from (32). If s is odd then we may use the even case we've just proved to obtain (28) from (32). The rest of the proposition follows quickly. □

Problem 6.4. Unfortunately, Prop. 6.3 tells us nothing when $s \equiv 1 \pmod p$. Maple computation reveals that for all such s and all primes $p < 10{,}000{,}000$ we have $(p-1)/2 \notin J(s|p)$ except $p = 1093$ and $p = 3511$. Are there any other such primes? Can one characterize all such primes?

The above proposition says that if s is even and $p - 1 \nmid s$ then $(p-1)/2 \in J_1(s|p)$. A natural question is that when is $(p-1)/2 \in J_1(s|p^2)$? The answer is given below.

Corollary 6.5. *Suppose s is a positive even integer such that $p-1 \nmid s$. Let n be the unique integer between 2 and $p-1$ such that $n-1 \equiv s \pmod{p-1}$. Then $H(s;(p-1)/2) \equiv 0 \pmod{p^2}$ if and only if either $(p, p-n)$ is an irregular pair or $p|2^n-1$. Moreover, when $p-1 \nmid s+2$ we have $H(s;(p-1)/2) \equiv 0 \pmod{p^3}$ if and only if $p^2|(2^n-1)B_{p-n}$.*

Proof. Let $m = (p-1)/2$. Prop. 6.3 implies that $\sum_{k=m+1}^{p-1} 1/k^{n+1} \equiv 0 \pmod p$ if $p - 1 \nmid s+2$.

$$\begin{aligned}H(s;m) = \sum_{k=m+1}^{p-1}\frac{1}{(p-k)^{n-1}} &\equiv \sum_{k=m+1}^{p-1}\frac{1}{k^{n-1}}+(n-1)p\sum_{k=m+1}^{p-1}\frac{1}{k^n} && \pmod{p^3}\\ &\equiv H(n-1;p-1)-H(n-1;m)+(n-1)pH(n;p-1)-(n-1)pH(n;m) && \pmod{p^3}.\end{aligned}$$

It follows from Thm. 1.1, [13, Thm. 2.4] and (28) that

$$2H(s;m) \equiv H(n-1;p-1)-(n-1)pH(n;m) \equiv pB_{p-n}\frac{(n-1)(2^n-1)}{n} \pmod{p^3}.$$

This finishes the proof of the corollary. □

Remark 6.6. For every positive even integer s and every irregular prime $p \ge s+4$ up to 100,000, p^2 always divides $H(s;(p-1)/2)$ exactly. Is this true in general? The answer is no. A calculation by Maple shows that for the 5952nd irregular pair $(p, p-n) = (130811, 52324)$ we have $n = 78487$ and $2^n \equiv 2 \pmod p$ and therefore $p^3|H(n-1;(p-1)/2)$. The peculiarity of this pair was already noticed in [5]. The next two such pairs are (599479,359568) (see [6]), and (2010401,1234960) (see [4]). Note that apparently this problem is not related to the problem of $2^p \equiv 2 \pmod{p^2}$.

Theorem 6.7. *Let s be a positive integer and $p > 2ds+1$ be an odd prime. Then*

$$\{p-1, j+(p-1)/2 : j=0,1,\cdots,d-1\} \subset J_1\big(\{2s\}^d|p\big).$$

Proof. Let $m=(p-1)/2$. By [13, Lemma 2.11] there are integers c_λ such that

$$d!H\big(\{s\}^d;n\big) = \sum_{\lambda\in P(d)} c_\lambda H_\lambda(s;n), \tag{33}$$

where $P(d)$ is the set of partitions of d, $H_{(\lambda_1,\dots,\lambda_r)}(s;n)=\prod_{l=1}^r H(\lambda_l s;n)$ and $c_{(d)}=(-1)^{d-1}(d-1)!$. Plugging in $n=m$ we get $m\in J_1\big(\{2s\}^d|p\big)$ by Prop. 6.3. By definition $H(\{s\}^d;q)=0$ for $q=1,\cdots,d-1$. When $q=1$ this implies that $\sum_{\lambda\in P(d)}c_\lambda=0$ by (33). Hence $m+1\in J_1\big(\{2s\}^d|p\big)$. Similarly, because 1, $1/2^{2s}$, $\cdots$, $1/(d-1)^{2s}$ are linearly independent when regarded as a function of s, we see that for all independent variables $x_1,\dots,x_j$, $j\le d-1$, we have

$$\sum_{\lambda=(\lambda_1,\dots,i\lambda_r)\in P(d)} c_\lambda \prod_{l=1}^r (x_1^{\lambda_l}+\cdots x_j^{\lambda_l})=0.$$

The theorem now follows from setting $x_j=1/(m+j)^{2s}$ for $j=1,\cdots,d-1$. □

Corollary 6.8. *Let s be a positive integer and $p>4s+1$ be an odd prime. Then*

(1) If s is even then $(p-1)/2, (p+1)/2\in J_1(s,s|p)$.

(2) If s is odd and $(p,p-s)$ is an irregular pair then $(p-1)/2\in J_1(s,s|p)$. Further, if s is odd, $2^s\not\equiv 2 \pmod p$, and $(p-1)/2\in J_1(s,s|p)$, then $(p,p-s)$ is an irregular pair. In particular, if $s\ge 3$ is odd and $p>2^s-2$ then $(p-1)/2\in J_1(s,s|p)$ if and only if $(p,p-s)$ is an irregular pair.

Proof. Let s and p be the integers satisfying the conditions of the corollary. When s is even the corollary follows from Thm. 6.7. If s is odd then by Prop. 6.3 and the shuffle relation we have

$$2H(s,s;(p-1)/2)\equiv H(s;(p-1)/2)^2 - H(2s;(p-1)/2). \tag{34}$$

The corollary follows immediately. □

7 Reserved set of partial sums of MZV series

In Conjecture B of [7] Eswarathasan and Levine state that there should be infinitely many primes p such that the divisible set $J(1|p)=\{0,p-1,p^2-p,p^2-1\}$. Boyd [2] further suggest $1/e$ as the expected density of such primes. The most important steps are to elucidate the structure of $J_1(1|p)$ and determine the relation between $J_t(1|p)$ and $J_{t+1}(1|p)$ for $t>0$. We put forward some similar results and conjectures concerning the divisible sets of general MZV series in this last section.

Definition 7.1. For any $\vec{s}\in\mathbb{N}^d$ there are finitely many function $f_0(x)=0, f_1(x),\dots,f_r(x)\in\mathbb{Q}[x]$ such that for all primes $p\ge wt(\vec{s})+3$

$$f_0(p)<f_1(p)<\cdots<f_r(p) \text{ and } f_0(p),f_1(p),\dots,f_r(p)\in J(\vec{s}|p).$$

We call the largest r the *reserved (divisibility) number* of MZV series $\zeta(\vec{s})$, denoted by $\rho(\vec{s})$. We call the corresponding set $\{f_0(x),\dots,f_{\rho(\vec{s})}(x)\}$ the *reserved (divisibility) set* of $\zeta(\vec{s})$, denoted by $RJ(\vec{s})=RJ(\vec{s};x)$. Its t-th segment is $RJ_t(\vec{s})=\{f(x)\in RJ(\vec{s}) : f(p)\le p^t-1 \text{ for all prime } p\}$ for $t\ge1$. Note that $0\in RJ_t(\vec{s})$ for all $t\ge0$. If $J(\vec{s}|p)=RJ(\vec{s};p)$ for some prime p then is called a *reserved prime* for MZV series $\zeta(\vec{s})$.

For example, the reserved number of the harmonic series is 3, the reserved set is $RJ(1)=\{0,x-1,x^2-x,x^2-1\}$, and 5 is a reserved prime for the harmonic series because $J(1|5)=\{0,4,20,24\}$. We summarize all known reserved sets in the following theorem.

Theorem 7.2. *Let $r,s,t,d\le 5$ be positive integers. Then*

1. $RJ(1)=\{0,x-1,x^2-1,x^2-x\}$.
2. If d is even then $RJ(\{1\}^d)=\{0,x-1,x,2x-1\}$.
3. If $1\neq d$ is odd then $RJ_{10}(\{1\}^d)=\{0,x-1\}$.
4. If $s\geq 3$ is odd then $RJ_{10}(\{s\}^d)=\{0,x-1\}$.
5. If s is even then $RJ_8(\{s\}^d)=\{0,i+(x-1)/2,x-1:0\leq i\leq d-1\}$.
6. If $s\geq 3$ is odd then $RJ(s,1)=\{0,x-1,x\}$.
7. If $s\neq t$ have the same parity and $t\neq 1$ then $RJ(s,t)=\{0,x-1\}$.
8. If s and t have different parity then $RJ(s,t)=\{0\}$.
9. If $r+s+t\geq 5$ is odd, $r,s,t\geq 2$, and $r\neq t$, then $RJ(r,s,t)=\{0\}$.
10. If s is odd then $RJ(r,s,r)=\{0,x-1\}$.
11. If $r+s+t\geq 6$ is even, $(r,s,t)\neq(4,3,5),(5,3,4)$, and $r,s,t\geq 2$ are not all the same, then $RJ(r,s,t)=\{0\}$.
12. $RJ_{10}(2,1,1)=RJ(1,1,2)=RJ(4,3,5)=RJ(5,3,4)=\{0,x-1\}$.
13. $RJ_{10}(1,2,1)=\{0,x-1,2x-1\}$.

Remark 7.3. We are sure that we can replace RJ_{10} in the above by RJ when more powerful computational tools are available to us.

Proof. Even without restriction of the bound 5, the inclusions $RJ(\vec{s};p)\subseteq J(\vec{s}|p)$ except the second and the last cases follow from equation (33), Thm. 1.1, [13, Thm. 3.1, Thm. 3.5], and Thm. 6.7.

For $\vec{s}=\{1\}^d$, $d\geq 2$, Thm. 1.1 implies $p-1\in J\big(\{1\}^m|p^{\mathrm{p}(m-1)}\big)$ for all $m\geq 1$ and $p\geq m+3$. In fact, we have

$$H(\{1\}^d;p-1)\equiv\frac{(-1)^{d-1}H(d;p-1)}{d}\equiv\begin{cases}-\dfrac{pB_{p-d-1}}{d+1} & \pmod{p^2}\quad \text{if } 2|d,\\ -\dfrac{p^2(d+1)B_{p-d-2}}{2d+4} & \pmod{p^3}\quad \text{if } 2\nmid d,\end{cases}\tag{35}$$

by [13, Thm 3.1]. So if $p\geq d+3$ then

$$H(\{1\}^d;p)=H(\{1\}^d;p-1)+\frac{1}{p}H(\{1\}^{d-1};p-1)\equiv\begin{cases}\dfrac{-p(d+2)B_{p-d-1}}{2(d+1)} & \pmod{p^2}\quad \text{if } 2|d,\\ -\dfrac{B_{p-d}}{d} & \pmod{p}\quad \text{if } 2\nmid d,\end{cases}\tag{36}$$

Further, setting $h_i=H(\{1\}^i;p-1)$, $h_0=1$ and $h_{-1}=0$ we have

$$\begin{aligned}H(\{1\}^d;2p-1)=&\sum_{i=0}^{d}\sum_{1\leq k_1<\cdots<k_i\leq p<k_{i+1}<\cdots<k_d<2p}\frac{1}{k_1k_2\dots k_d}\\ \equiv&\sum_{i=0}^{d}\Big(h_i+\frac{1}{p}h_{i-1}\Big)\Big(h_{d-i}+(-1)^{d-i}pH(d-i+1;p-1)\Big)\pmod{p^2}.\end{aligned}\tag{37}$$

Here we have used geometric series expansion inside $\mathbb{Q}_p$ such that for any $m<p$

$$\begin{aligned}\sum_{1\leq l_1<\cdots<l_m<p}\frac{1}{(p+l_1)\cdots(p+l_m)}\equiv&h_m-p\sum_{i=1}^{m}H\big((\{1\}^{i-1},2,\{1\}^{m-i});p-1\big)\pmod{p^3}\\ \equiv h_m+p((m+1)h_{m+1}-h_1h_m)\equiv&h_m+(-1)^m pH(m+1;p-1)\pmod{p^3}\end{aligned}$$

by equation (33). It follows from equations (33), (37) and [13, Thm. 3.1] that

$$H(\{1\}^d;2p-1)\equiv 2h_d+\frac{1}{p}\sum_{i=0}^{d-1}h_ih_{d-1-i}-(-1)^dH(d;p-1)\pmod{p^2}.$$

When d is even we have

$$H(\{1\}^d;2p-1)\equiv -\frac{(d+2)H(d;p-1)}{d}+\frac{2H(d-1;p-1)}{p(d-1)}\equiv -2pB_{p-d-1}\pmod{p^2}.\qquad(38)$$

So it's divisible by p. When $d=2n+1$ is odd $h_d\equiv 0\pmod{p^2}$ and we get

$$H(\{1\}^d;2p-1)\equiv\frac{1}{p}\sum_{i=0}^{n}h_{2i}h_{2n-2i}\equiv\frac{-H(2n;p-1)}{np}\equiv\frac{-2B_{p-d}}{d}\pmod{p}\qquad(39)$$

which is rarely congruent to 0.

For $RJ(1,2,1)$ we have for any prime $p\geq 7$

$$H(1,2,1;2p-1)=\sum_{1\leq l<m<n<2p}\frac{1}{lm^2n}=A+B+C+D,$$

where

$$\begin{aligned}
A&=\sum_{1\leq l<m<n\leq p}\frac{1}{lm^2n}=H(1,2,1;p-1)+\frac{1}{p}H(1,2;p-1),\\
B&=\sum_{1\leq l<m\leq p<n<2p}\frac{1}{lm^2n}=\left(H(1,2;p-1)+\frac{1}{p^2}H(1;p-1)\right)\sum_{1\leq k<p}\frac{1}{p+k},\\
C&=\sum_{1\leq l\leq p<m<n<2p}\frac{1}{lm^2n}=\left(H(1;p-1)+\frac{1}{p}\right)\sum_{1\leq m<n<p}\frac{1}{(p+m)^2(p+n)},\\
D&=\sum_{p<l<m<n<2p}\frac{1}{lm^2n}=\sum_{1\leq l<m<n<p}\frac{1}{(p+l)(p+m)^2(p+n)}\equiv H(1,2,1;p-1)\pmod{p}.
\end{aligned}$$

We know that $H(1,2,1;p-1)\equiv 0\pmod{p}$ by [13, Prop. 3.6] and $H(1;p-1)\equiv 0\pmod{p^2}$ by Wolstenholme's Theorem. By geometric series expansion we get

$$\sum_{1\leq m<n<p}\frac{1}{(p+m)^2(p+n)}\equiv\sum_{1\leq m<n<p}\frac{(1-2p/m)(1-p/n)}{m^2n}\pmod{p^2}.$$

Hence

$$H(1,2,1;2p-1)\equiv\frac{1}{p}\big(H(1,2;p-1)+H(2,1;p-1)\big)-2H(3,1;p-1)-H(2,2;p-1)\pmod{p}.$$

By Thm. 1.1 and [13, Thm. 3.1 or Cor. 3.4] we have $H(2,2;p-1)\equiv H(3,1;p-1)\equiv 0\pmod{p}$. Further, from shuffle relation we have

$$H(1,2;p-1)+H(2,1;p-1)=H(1;p-1)H(2;p-1)-H(3;p-1)\equiv 0\pmod{p^2}$$

by Thm. 1.1. This shows that $H(1,2,1;2p-1)\equiv 0\pmod{p}$.

To prove the theorem we now only need to demonstrate that $RJ(\vec{s};p)=J(\vec{s}|p)$ for some $p\geq \mathrm{wt}(\vec{s})+3$ which can be done through a case by case computation. We put this part of verification online [12]. In fact, much more data is available in this supplement. ∎

Problem 7.4. Are there any other $\vec{s}\in\mathbb{N}^d$ ($d\leq 3$) besides those listed in Thm. 7.2 such that $RJ(\vec{s})\neq\{0\}$?

We would be surprised to find an affirmative answer to this problem. When $d \geq 4$ we suspect that $RJ(\vec{s}) = \{0\}$ except when $\vec{s}$ is homogeneous or $\vec{s}$ is palindrome of odd weight (see [13, sec. 2.4 and sec. 3.2]), or $\vec{s}$ has one of the special forms listed in the last conjecture of [13].

From Thm. 7.2 we see that to determine $RJ(\vec{s})$ we often only need to study $RJ_1(\vec{s})$ because for all non-homogeneous $\vec{s}$ not equal to $(2r-1,1)$ or $(1,2,1)$, the proportion of primes p such that $J_t(\vec{s}|p) = \emptyset$ for all $t \geq 2$ is supposed to be positive. This implies that $RJ(\vec{s}) = RJ_1(\vec{s})$ for all such $\vec{s}$. Precisely, we have the following

Conjecture 7.5. *Suppose $\vec{s} \in \mathbb{N}^d$ such that (i) $\vec{s} = 1$, or (ii) $\vec{s} = (1,2,1)$, or (iii) $\vec{s} = (2r-1,1)$ for some $r \geq 1$, or (iv) $\vec{s} = \{1\}^{2d}$ for some $d \geq 1$. Then $RJ(\vec{s}) = RJ_2(\vec{s})$. For all other $\vec{s}$ we have $RJ(\vec{s}) = RJ_1(\vec{s})$.*

In what follows we provide a heuristic argument for part of this conjecture. It is not hard to prove the conjecture for each explicitly given $\vec{s}$ by some computation. But we could not prove the general statement.

(I) $d = 1$ and $s \geq 2$. Then $J_2(s|p) = \emptyset$ if $J_1(s|p^s) = \emptyset$ by Thm. 3.6. First let $s \geq 4$. By [13, Thm. 2.8] we know that when p is large enough higher than expected powers of p divides $H(s;p-1)$ occurs if and only if $p^2 | B_{p(p-1)-2n}$ for some irregular pairs $(p, p-2n-1)$ which rarely happens (here $s = 2n$ or $s = 2n-1$). So we can safely bet that the density of primes p such that $p^s | H(s;p-1)$ is 0. The same is true for $H(s;(p-1)/2)$ by Prop. 6.3 and Cor. 6.5. We further believe that when $r \neq (p-1)/2$ ranges from 1 to $p-2$ the numbers $H(s;r)$ distribute randomly modulo p^s. Therefore the probability of $J_1(s|p^s) = \emptyset$ is $(1-1/p^s)^{p-3} \to 1$ as $p \to \infty$. For $s = 2$ (resp. $s = 3$), the above argument fails only for irregular primes such that $(p, p-3)$ (resp. $(p, p-5)$) is an irregular pair, whose density is evidently 0. In a word, for any fixed positive integer $s \geq 2$, the proportion of p such that $J_2(s|p) \neq \emptyset$ is 0.

Further, by recursive relation (4) we find that if $n \in G_{t+1}$ is rooted on r, $1 \leq r \leq p-1$ (meaning that $n = pn_1 + r_1$, $n_1 = pn_2 + r_2$, $\dots$, $n_{t-1} = pn_t + r_{t-1}$ and $n_t = r$), and $p \nmid H(s;r)$ then $v_p\big(H(s;n)\big) = -s(t+1)$.

(II) $d \geq 2$ and $\vec{s} = \{1\}^d = \{1\}^{2m+1}$ for some $m \in \mathbb{N}$. For any prime $p \geq d+3$ we have for $n \in G_2$

$$H(\{1\}^{2m+1};n) = H(\{1\}^{2m+1};n-1) + \frac{1}{n} H(\{1\}^{2m};n-1). \tag{40}$$

The case $n = p+1$ can be safely excludes because it's clear that the other term, namely $H(\{1\}^{2m+1};p)/(p+1) \equiv -B_{p-2m-1}/(2m+1) \pmod{p}$, is rarely divisible by p by (36). The same reason applies to $n = p$, only this time the first term is always divisible by p while the second term rarely is. It is not hard to see that $H(\{1\}^{2m+1};n) \in \mathbb{Z}_p$ for all $p+1 < n < p+2m$. However,

$$\begin{aligned} H(\{1\}^d;p+d-1) \equiv & \frac{1}{p+d-1} H(\{1\}^{d-1};p+d-2) \equiv \cdots \qquad \pmod{\mathbb{Z}_p} \\ \equiv & \frac{1}{(p+d-1)\cdots(p+1)} H(1;p) \equiv \frac{1}{(d-1)!p} \pmod{\mathbb{Z}_p}. \end{aligned} \tag{41}$$

This means that $v_p\big(H(\{1\}^{2m+1};p+2m)\big) = -1$. If we assume random distribution of $pH(\{1\}^{2m+1};n)$ for all other $p+2m < n < 2p$ modulo p then the heuristic probability that none of $H(\{1\}^{2m+1};n)$ is divisible by p is about $(1-1/p^2)^{p-2m-1} \to 1$ as $p \to \infty$. Further it's not hard to show that in this range the v_p-valuation is bounded below by -1.

Turning to $n = 2p$ and using (38), (39) and (40) we find that $H(\{1\}^{2m+1};2p) \equiv -(2m+3)B_{p-2m-1}/(2m+1) \pmod{p}$. This implies that the density of p such that $2p \in J_2(\{1\}^{2m+1}|p)$ is probably 0 for any fixed m, in any case it's very small.

When $2p \leq n \leq 2p+2m-1$ it's easy to show that $v_p\big(H(\{1\}^{2m+1};n)\big) \geq -1$. When n passes $2p+2m-1$ things are quite different because we now usually have p^2 appearing in the denominator of $H(\{1\}^{2m+1};n)$. The chance for this number to be p-divisible is much smaller. Indeed, consider

$$\begin{aligned} H(\{1\}^{2m+1};2p+2m-1) \equiv & \frac{H(\{1\}^{2m};2p+2m-2)}{2p+2m-1} \equiv \cdots \qquad \pmod{\frac{1}{p}\mathbb{Z}_p} \\ \equiv & \frac{H(1,1;2p)}{(2p+2m)\cdots(2p+1)} \equiv \frac{H(1;2p-1)}{(2m)!2p} \equiv \frac{1}{2(2m)!p^2} \pmod{\frac{1}{p}\mathbb{Z}_p} \end{aligned}$$

since $H(1;2p-1)\equiv 1/p+2H(1;p-1)\equiv 1/p.\pmod{p\mathbb{Z}_p}$. This implies that $v_p\big(H(\{1\}^{2m+1};2p+2m-1)\big)=-2$. Similar but more involved argument shows that in general for $f=1,2,\dots,d$, $(d=2m+1)$ we have that

$$v_p\big(H(\{1\}^{2m+1};fp+2m-f+1)\big)=-f.$$

In each interval $fp+2m-f<n\le(f+1)p+2m-f$ we can safely assume the numbers $p^fH(\{1\}^{2m+1};n)$ distribute randomly modulo p. Then the probability that p divides some of them in this range is $(1-1/p^{f+1})^p\to 0$ as $p\to\infty$. The same argument applies to $dp+2m-d=(2m+1)p-1<n<p^2$ and we see that probability that p divides none of such n is $(1-1/p^{d+1})^{p^2-dp}\to 1$ as $p\to\infty$ because $d=2m+1\ge 3$.

(III) $d\ge 2$ and $\vec{s}=\{s\}^d$, $s\ge 2$. This case is easier than (II). We can use induction on d and the results from part (I). We leave out the details.

(IV) $d=2$ and $\vec{s}=(s_1,s_2)\ne(2r-1,1)$ for any $r\ge 1$ and $s_1\ne s_2$, or $d\ge 3$ and $\vec{s}\ne(1,2,1)$ is non-homogeneous. Then we believe that there does not exist recursive relations similar to (4). However, heuristically and inductively we can still show that if $n\in G_{t+1}$ and $t\ge 1$ then for almost all $p>d$

$$0\ge v_p\big(H(\vec{s};n)\big)\ge-\operatorname{wt}(\vec{s})\cdot t. \tag{42}$$

The second inequality is obvious because each term in $H(\vec{s};n)$ satisfies the same inequality. Only the left hand inequality is relevant to Conj. 7.5 and needs explanation.

We only consider G_2 as other segments G_t are easier. We divide G_2 into p parts: $[ap,(a+1)p-1]$ for $1\le a\le(p-1)$. We only need to consider the end points of these intervals because by using

$$H(\vec{s};n)=H(\vec{s};n-1)+\frac{H(\vec{s}\,';n-1)}{n^{s_d}},\quad \vec{s}\,'=(s_1,\dots,s_{d-1}),$$

we can easily reduce the case $ap^t<n<(a+1)p^t$ to the above. The case $n=ap$ in the above equation will play an very important role in our argument so we rewrite it here:

$$H(\vec{s};ap)=H(\vec{s};ap-1)+\frac{H(\vec{s}\,';ap-1)}{a^{s_d}p^{s_d}}. \tag{43}$$

(IV.1) Let $d=2$ and $\vec{s}=(s_1,s_2)\ne(2r-1,1)$ for any $r\ge1$ and $s_1\ne s_2$. First suppose $a=1$. There're two cases. (1) If $s_2\ge 3$, or $s_2=2$ and s_1 even then for almost all primes p we get

$$v_p\big(H(s_1,s_2;p)\big)-s_2=1-s_2=-1.$$

(2) If $s_2=2$ and s_1 is odd, or $s_2=1$ and s_1 is even, then $p\nmid H(s_1,s_2;p-1)$ whereas $p\nmid H(s_1;p-1)/p^{s_2}$ for almost all p by [13, Thm. 3.1] and [13, Prop. 2.4], respectively. The chance that their sum is divisible by p is $1/p$ for p large if we assume random distribution of these two numbers modulo p. So for almost all p

$$v_p\big(H(s_1,s_2;p)\big)=0.$$

Let's assume now $2\le a\le p-1$. Then by the congruence (12) of Lemma 3.5

$$H(s_1;ap-1)\equiv H(s_1;p-1)+\frac{1}{p^{s_1}}H(s_1;a-1)\pmod p.$$

For almost all p this has v_p value equal to $-s_1$ except when $a-1=(p-1)/2$ and s_1 is even in which case the value is increased by 1 for almost all primes p by Cor. 6.5 and Problem 6.4. By (43) this means that for $2\le a\le p-1$ and almost all p

$$v_p\big(H(s_1,s_2;ap)\big)\equiv\sum_{b=1}^{a}\frac{H(s_1;b-1)}{b^{s_2}p^{s_1+s_2}}\equiv\frac{H(s_1,s_2;a-1)}{p^{s_1+s_2}}\not\equiv 0\pmod{\frac{1}{p^{s_2}}\mathbb{Z}_p}$$

because $s_1\ne s_2$. This proves (42) for $d=2$ and $t=1$ for almost all p.

(IV.2) Assume now $d\ge3$ and $\vec{s}$ is non-homogeneous and assume (42) holds for smaller d's. In equation (43) if $a=1$ then $v_p\big(H(\vec{s}\,';ap-1)\big)\le 2$ for almost all p and the upper bound can be achieved only if $\vec{s}\,'$ is homogeneous of odd weight by shuffle relation (33). But the term $H(\vec{s};p-1)$

is assumed to be a random number modulo p so that with probability $1/p$ its v_p-valuation is 0. So $v_p\big(H(\vec{s};p)\big) \le 0$ whenever the two terms on the right hand side of (43) have different valuations. Otherwise, the probability of $v_p\big(H(\vec{s};p)\big) \ge 1$ is at most $1/p$ when assuming random distributions modulo p.

When $a \ge 2$ we assume that $H(\vec{s}\,';ap-1)$ has random distribution modulo p^2 (the case $a=2$ and $\vec{s}\,'=(1,2,1)$ has to be dealt with separately, but that's not hard). Thus the chance that $p|H(\vec{s};ap)$ is less than $1/p^3$ for large p. This implies that the probability of $J_2(\vec{s}|p)=\emptyset$ is roughly $(1-1/p^3)^{p^2} \to 1$ as $p\to\infty$.

Definition 7.6. Let $\vec{s}\in\mathbb{N}^d$. Define the *reserved density* of the MZV series $\zeta(\vec{s})$ by

$$\text{density}(RJ(\vec{s});X)=\frac{\sharp\{\text{prime } p:\text{wt}(\vec{s})+2<p<X, J(\vec{s}|p)=RJ(\vec{s})\}}{\sharp\{\text{prime } p:\text{wt}(\vec{s})+2<p<X\}} \tag{44}$$

and the mth *reserved density* by

$$\text{density}(RJ^m(\vec{s});X)=\frac{\sharp\{\text{prime } p:\text{wt}(\vec{s})+1<p<X, \cup_{t=0}^m J_t(\vec{s}|p)=RJ_m(\vec{s})\}}{\sharp\{\text{prime } p:\text{wt}(\vec{s})+2<p<X\}}. \tag{45}$$

Conjecture 7.7. *Let $\vec{s}\in\mathbb{N}^d$. Then*

$$\text{density}(RJ(\vec{s});\infty)=\begin{cases}1/\sqrt{e}, & \text{if } d=1, \vec{s}\ge 2,\\ 1/e, & \text{if } d=\vec{s}=1 \text{ or } d\ge 2.\end{cases}$$

Note that we always have $RJ(\vec{s};p)\subseteq J(\vec{s}|p)$. We have put the data strongly supporting Conj. 7.7 online [11]. In fact, we have only computed the first or the second reserved density because according to Conj. 7.5 this is enough to determine the reserved density in whole.

We now provide a heuristic argument for Conj. 7.7. Suppose $d=1$ and $\vec{s}=s\ge 2$ first. Then by Prop. 6.1 we only consider $H(s;r)$ for $1\le r\le (p-5)/2+\mathfrak{p}(s-1)$ because for most p the midpoint $(p-1)/2\in J_1(s|p)$ if and only if s is even (see Prop. 6.3). If we assume that when r varies the numbers $H(s;r)$ distribute randomly modulo p for any large fixed p then the probability that $J_1^0(s|p)=RJ_1(s;p)$ is $(1-1/p)^{(p-5)/2+\mathfrak{p}(s-1)}\to 1/\sqrt{e}$ as $p\to\infty$. By the argument in (I) after Conj. 7.5 we see that the probability that $J(s|p)=RJ(s;p)$ is $1/\sqrt{e}$.

Now we assume $d\ge 2$. In general $J_1^0(\vec{s}|p)$ does not have any symmetry so we see that the probability that $J_1^0(\vec{s}|p)=RJ_1(\vec{s};p)$ is $(1-1/p)^{p-\delta}\to 1/e$ as $p\to\infty$, where $\delta=\sharp RJ_1(\vec{s})$. When $\vec{s}$ does not belong to the cases (i)-(iv) in Conj. 7.5 we see that the probability that $J(\vec{s}|p)=RJ(\vec{s};p)$ is $1/e$ by Conj. 7.5.

Finally let's deal with larger reserved sets when $d\ge 2$. By Thm 7.2 we know that if $\vec{s}=\{1\}^{2m}$ or $(1,2,1)$ or $(2r-1,1)$ for some $r\ge 1$ then $RJ(\vec{s})=RJ_2(\vec{s})$. Let $\vec{s}=\{1\}^{2m}$. It follows from equation (41) that when $p+2m-1\le n<2p$ the probability that p divides $H(\{1\}^{2m};n)$ is $1/p^2$. Other heuristic argument of part (II) after Conj. 7.5 implies that $v_p\big(H(\{1\}^{2m};2p)\big)=-1$ for almost all prime p. As n gets large it's more and more *unlikely* that $n\in J(\{1\}^{2m}|p)$. We may thus disregard all $n\ge p+2m-1$. So assuming random distribution of numbers $H(\{1\}^{2m};n)$ modulo p for $2\le n\le p+2m-2$ we see that the probability that $J(\{1\}^{2m}|p)=RJ(\{1\}^{2m};p)$ is $(1-1/p)^{p+2m-5}\to 1/e$ as $p\to\infty$. We omit the arguments for $\vec{s}=(1,2,1)$ and $(2r-1,1)$ which are similar.

We conclude our paper by some conjectures which concern distributions of irregular primes in disguised forms.

Conjecture 7.8. *Let r, s and t be positive integers. Then*

1. *If $s>1$ is odd then there are infinitely many primes p such that $J_1(s|p)=\{(p-1)/2,p-1\}$.*
2. *If $s>1$ is odd then there are infinitely many primes p such that $J_1(s,s|p)=\{(p-1)/2,p-1\}$.*
3. *Let s,t be positive integers. Suppose $s+t$ is odd. Then there are infinitely many primes p such that $J_1(s,t|p)=\{p-1\}$.*

4. Let r, s, t be positive integers. Suppose $r+s+t$ is odd and $r \neq t$. Then there are infinitely many primes p such that $J_1(r, s, t|p) = \{p-1\}$.

Note that by various results of this paper and [13] an affirmative answer to any part of our Conj. 7.8 would imply that there are infinitely many irregular pairs $(p, p-w)$ for any fixed odd number w (≥ 5 in 4). Therefore, even if the sets of primes in Conj. 7.8 are expected to be infinite they are extremely sparse; very likely they have zero density.

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