IS $2d+1$ A GROWTH RATE OF THE RANK-d FREE GROUP? A POSITIVE ANSWER AT $d=3$, AND WHERE THE DIAGONAL CONSTRUCTION STOPS

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Abstract. For a group G with a finite generating set S, write $\mathrm{e}(G,S)=\lim_n |B_S(n)|^{1/n}$ for the exponential growth rate of the word metric, and $\xi(G)=\{\mathrm{e}(G,S) : S \text{ a finite generating set of } G\}$ for the growth spectrum. Fujiwara, Kim and Tanaka have recently determined the second and third smallest elements of $\xi(F_d)$ for the rank-d free group, and close their paper with the observation that $2d+1$ is an accumulation point of $\xi(F_d)$ which is attained at $d=2$, followed by the sentence "we do not know if $2d+1 \in \xi(F_d)$ for $d>2$" and the corresponding question. We answer it affirmatively at $d=3$: the generating set $S_\star=\{a,b,c,c^2,c^3\}$ of F_3 has spherical growth series $(1+t)(1+5t)/\big((1-7t)(1+3t)\big)$ and hence $\mathrm{e}(F_3,S_\star)=7$, so $7\in\xi(F_3)$; the generating set has the smallest cardinality, $d+2=5$, that any realisation of $2d+1$ can have. We also show that this is where the construction stops: calling S *diagonal* when it is a union $\bigcup_i\{a_i^k : k\in K_i\}$ of powers of the members of a free basis, a diagonal generating set of F_d has growth rate $2d+1$ if and only if $d\in\{2,3\}$, and at $d=3$ the set $S_\star$ is the only one up to relabelling. Deciding the question for $d\geq 4$ therefore requires a generating set that respects no free-product decomposition, and remains open. The value $\mathrm{e}(F_3,S_\star)=7$ and the general classification are proved by hand, from the classical free-product growth identity; they are not machine-checked, since the length formula they rest on has no formalisation. What is machine-checked in Lean 4 is the counting model behind them — its recurrence, its closed form, the two-sided bound $7^n\leq\sigma_n\leq 2\cdot 7^n$ and the resulting limit 7 — together with its agreement with the ball cardinalities $1, 11, 77, 551$ of F_3 computed inside the free group itself, and the whole Diophantine classification of the diagonal sets built from intervals.

1. Introduction

Growth rates and the growth spectrum. Let G be a group with a finite generating set S, and let $B_S(n)$ denote the set of elements of word length at most n with respect to S. Following the paper this one answers, we write

$$\mathrm{e}(G,S) \;:=\; \lim_{n\to\infty} |B_S(n)|^{1/n} \;\in\; [1,\, 2|S|-1],$$

the limit existing by submultiplicativity, and

$$\xi(G) \;:=\; \{\, \mathrm{e}(G,S) \;:\; S \text{ is a finite generating set of } G\,\},$$

the *growth spectrum* of G. Fujiwara and Sela [3] proved that $\xi(G)$ is well-ordered in $\mathbb{R}$ for a non-elementary hyperbolic group G, with order type at least ω^ω; in particular $\xi(G)$ has a minimum, answering a question of de la Harpe [5]. For the free group F_d of rank $d\geq 2$ the order type is exactly ω^ω [3], and the minimum is $\mathrm{e}_1(F_d)=2d-1$, achieved by a free basis [5]. We refer to [8] for an exposition of [3], and to [4] for the wider circle of growth problems.

The source and its question. Fujiwara, Kim and Tanaka [2] determine the next two values,

$$\mathrm{e}_2(F_d)=d-1+\sqrt{d^2+4d-4}, \qquad \mathrm{e}_3(F_d)=\frac{2d-1+\sqrt{4d^2+12d-15}}{2},$$

for every $d\geq 2$, and identify the generating sets that realise them. Their closing section records that $2d+1$ is an accumulation point of $\xi(F_d)$ from below, by a small cancellation argument of Shukhov [11], that a smaller accumulation point $\alpha_d(1,+\infty):=d+\sqrt{d^2+2d-3}$ is known and lies in $\xi(F_d)$, and then, verbatim ([2], §6; the displayed question is Question 6.2 there):

As noted above, $2d+1$ is an accumulation point of $\xi(F_d)$. Observe that $5 \in \xi(F_2)$ when $d = 2$; indeed, by a direct computation, $\mathrm{e}(F_2, \{a_1, a_1^2, a_2, a_2^2\}) = 5$. However, we do not know if $2d+1 \in \xi(F_d)$ for $d > 2$.

Question. Does $2d+1$ belong to $\xi(F_d)$ for every $d > 2$?

The paper prints no value of e at any generating set of F_d for $d \geq 3$. The natural first guess — that the $d = 2$ example generalises as $S = \{a_1, a_1^2, \dots, a_d, a_d^2\}$ — is false: that set has growth rate $4d-3$, which equals $2d+1$ only at $d = 2$ (Proposition 3.4). At $d = 3$ it gives 9, not 7. This failure is presumably why the question is asked.

What is settled here. Call a generating set of F_d *diagonal* with respect to a free basis $a_1, \dots, a_d$ when it has the form

$$S \;=\; \bigcup_{i=1}^{d} \{\, a_i^k \;:\; k \in K_i \,\}, \qquad K_i \subset \mathbb{Z}_{>0} \text{ finite},\ \gcd K_i = 1.$$

For such a set the word length is additive over the syllables of the free-product normal form of $F_d = \langle a_1 \rangle * \cdots * \langle a_d \rangle$, so the growth series is a computable rational function and the question "is $\mathrm{e}(F_d, S) = 2d+1$?" collapses to a single equality of rational numbers (Section 2). Three things follow.

First, the answer to the question is *yes* at $d = 3$.

Theorem A (Theorem 4.1). $\mathrm{e}(F_3, \{a, b, c, c^2, c^3\}) = 7 = 2 \cdot 3 + 1$; hence $7 \in \xi(F_3)$. The spherical growth series of F_3 with respect to this generating set is $(1+t)(1+5t)/\big((1-7t)(1+3t)\big)$, its ball sizes are $1, 11, 77, 551, 3833, 26915, 188165, \dots$, and the generating set has the smallest cardinality, $d + 2 = 5$, that any realisation of $2d+1$ in $\xi(F_d)$ can have (Proposition 4.2).

Second, the diagonal construction stops there.

Theorem B (Theorem 5.4). A diagonal generating set S of F_d satisfies $\mathrm{e}(F_d, S) = 2d+1$ if and only if $d \in \{2, 3\}$. For $d = 3$ the only such S is $\{a, b, c, c^2, c^3\}$, up to relabelling the free basis.

Third — and this is what keeps the question open — a generating set of F_d, $d \geq 4$, realising $2d+1$ would have to be non-diagonal, so that no free-product decomposition of F_d is compatible with it and the growth series has to be extracted from a geodesic automaton rather than from a product formula. Section 7 explains why a breadth-first numerical screen cannot substitute for that.

Restricted to the sets built from intervals $K_i = \{1, 2, \dots, m_i\}$ — the shape of every example in [2] — the criterion becomes the Diophantine equation

$$\sum_{i=1}^{d} \frac{1}{d + m_i} \;=\; \frac{d-1}{d},$$

whose solution set in positive integers is determined completely (Theorems 5.7 and 5.8): for $d \geq 4$ it is empty, and at $d = 3$ the unique solution is $(m_1, m_2, m_3) = (1, 1, 3)$, which is exactly $\{a, b, c, c^2, c^3\}$.

We also record two realisations of $5 \in \xi(F_2)$ beyond the one in [2] (Proposition 6.1), one of which is not built from an interval and so is invisible to the equation above.

What is proved by hand and what is machine-checked. The distinction matters here, and we keep it explicit throughout. Theorem A, Theorem B and Proposition 4.2 are proved in the ordinary mathematical sense, from the classical free-product growth identity of Section 2; they are not part of the formal development, because the length formula they rest on — that the word length of a diagonal generating set is additive over free-product syllables — has no formalisation, and no proof assistant library known to us carries growth series of groups at all. What is formalised and machine-checked in Lean 4 is: the counting model whose growth rate is the value in Theorem A, including its recurrence, its closed form, the two-sided bound $7^n \leq \sigma_n \leq 2 \cdot 7^n$ and the resulting limit 7 in the definition of e above (Theorem 4.3); the exact word-metric ball cardinalities of F_2 and

F_3 for the four generating sets discussed, computed inside the free group and matched against the model term by term (Theorem 4.3, Proposition 3.1, Proposition 3.4, Proposition 6.2); and the full solution of the Diophantine equation above (Theorems 5.7 and 5.8). Section 8 says precisely which statements carry which status.

2. Preliminaries

Balls, spheres and growth series. Throughout, a generating set S of a group G is finite and the word metric is taken with respect to $S \cup S^{-1}$, so that $B_S(n)$ is the set of products of at most n elements of $S \cup S^{-1}$ and $|g|_S$ is the least such n. The cardinality $|S|$ in the range $\mathrm{e}(G,S) \in [1, 2|S|-1]$ of [2] is that of S itself, not of its symmetrisation; as in [2, Remark 1.2], S is normalised so that $1 \notin S$ and exactly one element of each pair $\{s, s^{-1}\}$ is kept, so that $|S \cup S^{-1}| = 2|S|$. Write $\sigma_S(n) = |B_S(n)| - |B_S(n-1)|$ for the sphere sizes and

$$\Sigma_{G,S}(t) \;=\; \sum_{g\in G} t^{|g|_S} \;=\; \sum_{n\ge 0} \sigma_S(n)\, t^n$$

for the spherical growth series. Since $|B_S(n)|$ is submultiplicative, $\mathrm{e}(G,S)$ exists, and it is the reciprocal of the radius of convergence of $\Sigma_{G,S}$ ([2, Lemma 2.1(1)], whose proof refers to [5, VI.A and VI.C]); as the coefficients are non-negative, that radius is itself a singularity of the series, by Pringsheim's theorem.

Cyclic factors. For a finite $K \subset \mathbb{Z}_{>0}$ with $\gcd K = 1$, the set K generates $\mathbb{Z}$; write $\ell_K(n)$ for the word length of $n \in \mathbb{Z}$ with respect to K, that is, the least number of elements of $K \cup (-K)$ summing to n. Then $\ell_K(-n) = \ell_K(n)$, so

$$\Sigma_{\mathbb{Z},K}(t) \;=\; 1 + 2\,u_K(t), \qquad u_K(t) \;:=\; \sum_{n\ge 1} t^{\,\ell_K(n)}.$$

It is convenient to count by length rather than by value. Put

$$C_j(K) \;:=\; \#\{\, n \ge 1 \;:\; \ell_K(n) \le j \,\},$$

a finite number, since $\ell_K(n) \le j$ forces $n \le jM$, where $M := \max K$. Abel summation gives

$$u_K(t) \;=\; (1-t)\sum_{j\ge 1} C_j(K)\, t^{\,j} \qquad (0 \le t < 1), \tag{1}$$

convergent because $C_j(K) \le jM$. Two further facts are used throughout. First, $\ell_K(jM) = j$ for every $j \ge 1$: it is at most j by using M j times, and at least j because a sum of fewer than j elements of $K \cup (-K)$ has absolute value less than jM. Hence $C_j(K) \ge j$ and

$$u_K(t) \;\ge\; \sum_{j\ge 1} t^{\,j} \;=\; \frac{t}{1-t} \qquad (0 \le t < 1). \tag{2}$$

Second, $\ell_K(n+M) = \ell_K(n) + 1$ for all sufficiently large n. Indeed, put $h(n) := M\,\ell_K(n) - n$. Every element of $K \cup (-K)$ has absolute value at most M, so $\ell_K(n) \ge n/M$ and $h(n) \ge 0$; and $\ell_K(n+M) \le \ell_K(n) + 1$ gives $h(n+M) \le h(n)$. Thus along each residue class modulo M the sequence h is a non-increasing sequence of non-negative integers, hence eventually constant, and $h(n+M) = h(n)$ says exactly that $\ell_K(n+M) = \ell_K(n) + 1$. For large j each residue class modulo M therefore contributes exactly one n with $\ell_K(n) = j$, so $C_{j+1}(K) = C_j(K) + M$; in particular ℓ_K is determined by finitely many values and u_K is a rational function of t, which is how we evaluate it in exact arithmetic.

For an interval $K = \{1, 2, \ldots, m\}$ one has $\ell_K(n) = \lceil n/m \rceil$, hence $C_j(K) = mj$ and

$$u_K(t) = \frac{mt}{1-t}, \qquad \Sigma_{\mathbb{Z},K}(t) = \frac{1 + (2m-1)t}{1-t}. \tag{3}$$

The free-product identity, and the realisability criterion.

Proposition 2.1. *Let $G = G_1 * \cdots * G_r$ and let $S = S_1 \sqcup \cdots \sqcup S_r$ with S_i a finite generating set of G_i. Then*

$$\frac{1}{\Sigma_{G,S}(t)} \;=\; \sum_{i=1}^{r} \frac{1}{\Sigma_{G_i,S_i}(t)} \;-\; (r-1).$$

Proof. Because S is a union of generating sets of the factors, the word length of $g \in G$ is the sum of the word lengths of the syllables of its free-product normal form. For $r = 2$, write $\varsigma_i := \Sigma_{G_i,S_i} - 1$, the series of the non-trivial elements of G_i. Grouping the elements of $G_1 * G_2$ by their alternating normal form gives

$$\Sigma_{G,S} = \frac{1 + \varsigma_1 + \varsigma_2 + \varsigma_1\varsigma_2}{1 - \varsigma_1\varsigma_2} = \frac{(1+\varsigma_1)(1+\varsigma_2)}{1 - \varsigma_1\varsigma_2},$$

whence $\Sigma_{G_1,S_1}^{-1} + \Sigma_{G_2,S_2}^{-1} - 1 = (1 - \varsigma_1\varsigma_2)/\big((1+\varsigma_1)(1+\varsigma_2)\big) = \Sigma_{G,S}^{-1}$. The general case follows by induction on r. □

The identity is classical. For $r = 2$ it is [2, Lemma 2.1(2)], recorded there in the equivalent form $1 - \Sigma_{G,S}^{-1} = \big(1 - \Sigma_{G_1,S_1}^{-1}\big) + \big(1 - \Sigma_{G_2,S_2}^{-1}\big)$ with the proof referred to [5, VI.A and VI.C]; the argument above is included so that the induction on r, which is what we use, is self-contained.

Corollary 2.2. *Let $S = \bigcup_{i=1}^{d} \{a_i^k : k \in K_i\}$ be a diagonal generating set of F_d and put $x_0 := 1/(2d+1)$. Then*

$$\mathrm{e}(F_d, S) = 2d+1 \qquad \Longleftrightarrow \qquad \sum_{i=1}^{d} \frac{1}{1 + 2\,u_{K_i}(x_0)} \;=\; d-1.$$

Proof. Since $F_d = \langle a_1 \rangle * \cdots * \langle a_d \rangle$ and S is the union of the generating sets K_i of the factors, Proposition 2.1 applies and gives $1/\Sigma_{F_d,S}(t) = \Phi(t)$, where $\Phi(t) := \sum_i \big(1 + 2u_{K_i}(t)\big)^{-1} - (d-1)$. By (1) each u_{K_i} is finite, continuous and strictly increasing on $[0,1)$, so Φ is continuous and strictly decreasing there, with $\Phi(0) = d - (d-1) = 1$; and $u_{K_i}(t) \to \infty$ as $t \to 1^-$ by (2), so $\Phi(t) \to -(d-1) < 0$. Hence Φ has a unique zero $t_0 \in (0,1)$, and $\Phi > 0$ on $[0, t_0)$. Let R be the radius of convergence of $\Sigma_{F_d,S}$. On $[0,R)$ the series equals $1/\Phi$ and is at least 1, so $\Phi > 0$ there and $R \le t_0$. Conversely, Φ is a rational function with no zero on $[0, t_0)$, so $1/\Phi$ has no singularity there; since $\Sigma_{F_d,S}$ has non-negative coefficients, its radius of convergence is a singularity of it by Pringsheim's theorem, whence $R \ge t_0$. Thus $R = t_0$ and $\mathrm{e}(F_d,S) = 1/t_0$, so $\mathrm{e}(F_d,S) = 2d+1$ if and only if $\Phi(x_0) = 0$. □

By (3), when every K_i is an interval $\{1, \ldots, m_i\}$ one has $u_{K_i}(x_0) = m_i/(2d)$ and hence $\big(1 + 2u_{K_i}(x_0)\big)^{-1} = d/(d+m_i)$, so the criterion of Corollary 2.2 becomes the Diophantine equation

$$\sum_{i=1}^{d} \frac{1}{d+m_i} \;=\; \frac{d-1}{d}, \qquad m_i \in \mathbb{Z}_{\ge 1}. \tag{4}$$

3. The source's own values, and the first guess

Before proving anything new we reproduce, by our own computation, the data that [2] prints. The ball cardinalities below are obtained by enumerating reduced words inside the free group itself, not in any counting model.

Proposition 3.1. *Let $S = \{a_1, a_1^2, a_2, a_2^2\}$ in F_2, the generating set of [2] realising $5 \in \xi(F_2)$. Its symmetrisation has 8 elements, and*

$$|B_S(n)| \;=\; 1,\; 9,\; 49,\; 249 \qquad (n = 0,1,2,3),$$

which is $2 \cdot 5^n - 1$*; the sphere sizes are* $1, 8, 40, 200$*. These agree with the spherical growth series* $(1+3t)/(1-5t)$ *predicted for* S *by Proposition 2.1, and hence with the value* $\mathrm{e}(F_2, S) = 5$ *stated in* [2].

Remark 3.2. The sphere sequence $1, 8, 40, 200, 1000, 5000, \dots$ is entry A128625 of the On-Line Encyclopedia of Integer Sequences, described there as the expansion of $(1+3x)/(1-5x)$ [10] — an independent confirmation of the series that Proposition 2.1 predicts for this set.

Remark 3.3. Outside the formal development, the same breadth-first computation over freely reduced words reproduces three further values recorded in [2]: the sphere ratios for $\{a, a^2, b\}$ converge to $1 + 2\sqrt{2} = 3.8284\dots$ and those for the non-diagonal $\{a, ab, b\}$ to 4, the two values recorded in [2, Example 1.4]; and the ratios for $\{a, a^3, b\}$ converge to 4, which [2] asserts as $\mathrm{e}_3(F_2)$ in two printed statements taken together ([2, Theorem 1.1(2)] evaluates $\mathrm{e}_3(F_2) = 4$, and [2, Remark 1.2] lists $\{a_1, a_1^3, a_2, \dots, a_d\}$ among the sets realising $\mathrm{e}_3(F_d)$). The set $\{a, ab, b\}$ is not diagonal, so that reproduction also validates the computation where no product formula applies.

The obvious way to carry the $d = 2$ example to higher rank fails.

Proposition 3.4. *For every* $d \geq 2$*,*

$$\mathrm{e}\big(F_d,\ \{a_1, a_1^2, a_2, a_2^2, \dots, a_d, a_d^2\}\big) \ = \ 4d - 3,$$

and $4d - 3 = 2d + 1$ *if and only if* $d = 2$*. At* $d = 3$ *the ball cardinalities of this set, computed inside* F_3*, are* $1, 13, 121, 1093$ *for* $n = 0, 1, 2, 3$*, with sphere sizes* $1, 12, 108, 972$*; the growth rate is* 9*, not* 7*.*

Proof. Each factor carries $K = \{1, 2\}$, so (3) gives $u_K(t) = 2t/(1-t)$ and $\Sigma_{\mathbb{Z},K}(t) = (1+3t)/(1-t)$. Proposition 2.1 then yields

$$\frac{1}{\Sigma_{F_d,S}(t)} = d\,\frac{1-t}{1+3t} - (d-1) = \frac{1-(4d-3)t}{1+3t}, \qquad \Sigma_{F_d,S}(t) = \frac{1+3t}{1-(4d-3)t},$$

so $\sigma_S(n) = 4d\,(4d-3)^{n-1}$ for $n \geq 1$ and $\mathrm{e} = 4d - 3$. The equivalence $4d - 3 = 2d + 1 \Leftrightarrow d = 2$ is immediate. The stated $d = 3$ cardinalities are computed in F_3. ☐

So the coincidence at $d = 2$ in [2] is exactly a coincidence: the set $\{a_i, a_i^2\}_{i \leq d}$ realises $2d+1$ only in the one rank where $4d - 3$ and $2d + 1$ agree.

4. The answer at $d = 3$

Write $S_\star := \{a, b, c, c^2, c^3\} \subset F_3$, where $\{a, b, c\}$ is a free basis. It is diagonal, with $K_1 = K_2 = \{1\}$ and $K_3 = \{1, 2, 3\}$, and it generates F_3.

Theorem 4.1. $\mathrm{e}(F_3, S_\star) = 7 = 2 \cdot 3 + 1$*. Consequently* $7 \in \xi(F_3)$*: the question of* [2] *has a positive answer at* $d = 3$*. The spherical growth series is*

$$\Sigma_{F_3,S_\star}(t) \ = \ \frac{(1+t)(1+5t)}{(1-7t)(1+3t)}.$$

Proof. By (3), $\Sigma_{\mathbb{Z},\{1\}}(t) = (1+t)/(1-t)$ and $\Sigma_{\mathbb{Z},\{1,2,3\}}(t) = (1+5t)/(1-t)$. Proposition 2.1 gives

$$\frac{1}{\Sigma_{F_3,S_\star}(t)} = 2\,\frac{1-t}{1+t} + \frac{1-t}{1+5t} - 2 = \frac{1-4t-21t^2}{(1+t)(1+5t)} = \frac{(1-7t)(1+3t)}{(1+t)(1+5t)},$$

and inverting yields the stated series. The zeros of the numerator $1 - 4t - 21t^2$ are $1/7$ and $-1/3$; by the argument of Corollary 2.2 the unique zero in $(0,1)$ of $t \mapsto 2(1-t)/(1+t) + (1-t)/(1+5t) - 2$, namely $1/7$, is the radius of convergence of $\Sigma_{F_3,S_\star}$. Hence $\mathrm{e}(F_3, S_\star) = 7$. Equivalently, in the form of Corollary 2.2: $u_{\{1\}}(1/7) = 1/6$ and $u_{\{1,2,3\}}(1/7) = 1/2$, so $\frac{3}{4} + \frac{3}{4} + \frac{1}{2} = 2 = d - 1$ at $x_0 = 1/7$. ☐

Proposition 4.2. *If* S *is a finite generating set of* F_d *with* $\mathrm{e}(F_d, S) = 2d + 1$*, then* $|S| \geq d + 2$*. In particular* $|S_\star| = 5 = 3 + 2$ *is smallest possible at* $d = 3$*, as is* $|\{a_1, a_1^2, a_2, a_2^2\}| = 4 = 2 + 2$ *at* $d = 2$*.*

Proof. From $\mathrm{e}(F_d, S) \le 2|S| - 1$ we get $|S| \ge d+1$. Suppose $|S| = d+1$. Then $\mathrm{e}(F_d, S) = 2d+1 = 2|S| - 1$, the largest value the range permits; by a theorem of Koubi [6], the growth rate of a group with respect to a k-element generating set X equals $2k-1$ if and only if the group is free on X. So S would be a free basis of F_d of cardinality $d+1$, making F_d free of rank $d+1$, which it is not. Hence $|S| \ge d+2$. ☐

Theorem 4.1 is a statement about the group, obtained from Proposition 2.1, and it is not part of the formal development. Its counterpart there is the following, which pins the growth rate of the counting model at exactly 7 and checks the model against the group as far as the enumeration reaches.

Theorem 4.3. *Define $\sigma_0 = 1$, $\sigma_1 = 10$, $\sigma_2 = 66$ and*

$$\sigma_{n+2} \;=\; 4\,\sigma_{n+1} + 21\,\sigma_n \qquad (n \ge 1),$$

the sphere counts predicted for $S_\star$ by Theorem 4.1, and let $\beta_n = \sum_{k=0}^{n} \sigma_k$. Then:

(i) $105\,\sigma_n = 144 \cdot 7^n - 14\,(-3)^n$ *for every* $n \ge 1$*;*
(ii) $7^n \le \sigma_n \le 2 \cdot 7^n$ *for every* $n \ge 1$*;*
(iii) $\lim_{n\to\infty} \beta_n^{1/n} = 7$*, that is, the model has growth rate exactly* 7 *in the sense of the definition of* e*;*
(iv) $S_\star \cup S_\star^{-1}$ *has* 10 *elements and is closed under inversion,* $S_\star$ *generates* F_3*, and the word-metric ball cardinalities of* F_3 *with respect to* $S_\star$*, computed inside the free group, are*

$$|B_{S_\star}(n)| \;=\; 1,\; 11,\; 77,\; 551 \qquad (n = 0, 1, 2, 3),$$

which is β_n *for those* n.

Proof sketch. Parts (i) and (ii) are two-step inductions on the recurrence, with the two base cases $n = 1, 2$ checked against $\sigma_1 = 10$ and $\sigma_2 = 66$; the two roots 7 and -3 of $x^2 = 4x + 21$ are the reciprocals of the poles $1/7$ and $-1/3$ of the series in Theorem 4.1. Part (iii) is a squeeze: (ii) gives $7^n \le \beta_n$ for $n \ge 1$ and, summing, $\beta_n \le 7^{n+1}$ for all n, so $\beta_n^{1/n}$ is trapped between 7 and $7^{(n+1)/n} \to 7$. Part (iv) is a finite computation and is the only part that rests on exhaustive enumeration: for each $n \le 3$ the set of products of at most n elements of $S_\star \cup S_\star^{-1}$ is enumerated in the free group F_3, as reduced words, and its cardinality is compared with β_n. The enumeration is exhaustive at radius 3, where it visits 551 elements; the radii 4 and 5 (with 3833 and 26915 elements) were computed outside the formal development and agree with β_4 and β_5, and the sphere sizes there, 3282 and 23082, agree with σ_4 and σ_5. ☐

Remark 4.4. Part (iv) is what ties the model to the group at small radius; the statement that the agreement continues for every n is exactly the free-product length formula used in Proposition 2.1, and is the ingredient of Theorem 4.1 that is not formalised.

Remark 4.5. In the landscape of [2], the value 7 is an accumulation point of $\xi(F_3)$ from below, and the largest value smaller than 7 for which [2] gives a closed form is $\alpha_3(1, +\infty) = 3 + \sqrt{12} = 6.4641\ldots$; the two other closed forms [2] gives below 7, namely $\mathrm{e}_2(F_3) = 2 + \sqrt{17} = 6.1231\ldots$ and $\mathrm{e}_3(F_3) = (5 + \sqrt{57})/2 = 6.2749\ldots$, are smaller. Theorem 4.1 says that this accumulation point is itself attained.

5. Where the diagonal construction stops

Fix $d \ge 3$, write $x_0 = 1/(2d+1)$, and abbreviate $\tau(K) := \bigl(1 + 2u_K(x_0)\bigr)^{-1}$, so that Corollary 2.2 reads $\sum_i \tau(K_i) = d - 1$. From (3) with $m = 1$, $u_{\{1\}}(x_0) = 1/(2d)$ and $\tau(\{1\}) = d/(d+1)$. Setting $\delta(K) := d/(d+1) - \tau(K)$, the criterion becomes

$$\sum_{i=1}^{d} \delta(K_i) \;=\; \frac{d^2}{d+1} - (d-1) \;=\; \frac{1}{d+1}. \tag{5}$$

Lemma 5.1. *$C_j(K) \ge |K|\, j$ for every finite $K \subset \mathbb{Z}_{>0}$ and every $j \ge 1$. Consequently $u_K(x_0) \ge |K|/(2d)$, and $\delta(K) \ge 0$ with equality only for $K = \{1\}$.*

Proof. Let $M = \max K$ and $R_j = \{n \ge 1 : \ell_K(n) \le j\}$, so $C_j(K) = |R_j|$ and $R_j \subseteq [1, jM]$. For each $k \in K$ the number $(j-1)M+k$ lies in R_j and exceeds $(j-1)M \ge \max R_{j-1}$, so $|R_j| \ge |R_{j-1}|+|K|$; with $|R_1| = |K|$ this gives $C_j(K) \ge |K|j$. Substituting into (1) and summing $\sum_j j\, x_0^j = x_0/(1-x_0)^2$ gives $u_K(x_0) \ge |K|x_0/(1-x_0) = |K|/(2d)$; the last claim follows because $\gcd K = 1$ forces $K = \{1\}$ when $|K| = 1$. $\square$

Remark 5.2. The counting device in this proof — the $|K|$ elements $(j-1)M+k$, $k \in K$, new at level j — is the one used in [2, Lemma 2.3] at $|K| = 2$ and $|K| \ge 3$ to bound $\Sigma_{\mathbb{Z},K}$ from below by $\Sigma_{\mathbb{Z},\{1,2\}}$ and by $\Sigma_{\mathbb{Z},\{1,3\}}$ respectively. Lemma 5.1 is its extension to arbitrary $|K|$, in the form we need.

Lemma 5.3. *If $|K| = 2$ then $C_j(K) \le j^2 + j$ for every $j \ge 1$, and hence $u_K(x_0) \le (2d+1)/(2d^2)$.*

Proof. Write $K = \{p, q\}$. Every n with $\ell_K(n) \le j$ is c_1p+c_2q for some $(c_1, c_2) \in \mathbb{Z}^2$ with $|c_1|+|c_2| \le j$, and there are $2j^2 + 2j + 1$ such lattice points. The value map is odd, so the points of positive value are in bijection with those of negative value, and the origin has value 0; hence at most $\big((2j^2 + 2j + 1) - 1\big)/2 = j^2 + j$ distinct positive values occur. Substituting into (1) and summing $\sum_j (j^2 + j)\, t^j = 2t/(1-t)^3$ gives $u_K(x_0) \le 2x_0/(1-x_0)^2 = (2d+1)/(2d^2)$. $\square$

Theorem 5.4. *Let $S = \bigcup_{i=1}^d \{a_i^k : k \in K_i\}$ be a diagonal generating set of F_d.*

(i) *If $d \ge 4$, then $\mathrm{e}(F_d, S) \ne 2d+1$.*
(ii) *If $d = 3$ and $\mathrm{e}(F_3, S) = 7$, then $\{K_1, K_2, K_3\} = \{\{1\}, \{1\}, \{1, 2, 3\}\}$ as a multiset; that is, $S = S_\star$ up to relabelling the free basis.*

Together with the example of [2] *at $d = 2$, a diagonal generating set of F_d has growth rate $2d+1$ if and only if $d \in \{2, 3\}$.*

Proof. Let $d \ge 3$ and suppose $\mathrm{e}(F_d, S) = 2d+1$, so that (5) holds.

Step 1: at most one $K_i \ne \{1\}$. If $|K| \ge 2$ then Lemma 5.1 gives $u_K(x_0) \ge 1/d$, so $\tau(K) \le d/(d+2)$ and $\delta(K) \ge d/\big((d+1)(d+2)\big)$. Two indices with $K_i \ne \{1\}$ would give $\sum_i \delta(K_i) \ge 2d/\big((d+1)(d+2)\big)$, which exceeds $1/(d+1)$ exactly when $2d > d+2$, that is when $d > 2$. So for $d \ge 3$ there is at most one such index, and by (5) it satisfies $\delta(K) = 1/(d+1)$, i.e. $\tau(K) = (d-1)/(d+1)$, i.e.

$$u_K(x_0) \;=\; \frac{1}{d-1}. \tag{6}$$

(There is at least one such index, since $\sum_i \delta(K_i) = 1/(d+1) \ne 0$.)

Step 2: $|K| \le 3$, and $|K| \le 2$ for $d \ge 5$. Each $k \in K$ has $\ell_K(k) = 1$, so $u_K(x_0) \ge |K|\, x_0$; with (6) this gives $|K| \le (2d+1)/(d-1)$, which is < 4 for $d \ge 3$ and < 3 for $d \ge 5$.

Step 3: $|K| = 2$ is impossible. By Lemma 5.3, $u_K(x_0) \le (2d+1)/(2d^2)$, and $(2d+1)/(2d^2) < 1/(d-1)$ for every d, because $(2d+1)(d-1) = 2d^2 - d - 1 < 2d^2$. This contradicts (6).

Step 4: $|K| = 3$. Since $\gcd K = 1$, the case $|K| = 1$ would give $K = \{1\}$, which is excluded; so by Steps 2 and 3 the only possibility left is $|K| = 3$, and $d \le 4$. Lemma 5.1 gives $u_K(x_0) \ge 3/(2d)$, and (6) requires $3/(2d) \le 1/(d-1)$, i.e. $3(d-1) \le 2d$, i.e. $d \le 3$. For $d \ge 4$ this is a contradiction, which with Steps 2 and 3 proves (i).

For $d = 3$ the inequality of Step 4 is an equality, so the inequality of Lemma 5.1 is an equality for every j: $C_j(K) = 3j$ for all $j \ge 1$. Write $K = \{p < q < r\}$. Then $C_2(K) = 6$, while $R_2 \supseteq K \cup \{p+r,\ q+r,\ 2r\}$, and the three added numbers are distinct and exceed r, so this union already has six elements and $R_2 = K \cup \{p+r, q+r, 2r\}$. The positive numbers $q-p$, $r-p$, $r-q$ all lie in R_2 and are $< r$, so each lies in $R_2 \cap [1, r) = \{p, q\}$. From $q - p < q$ we get $q - p = p$, so $q = 2p$; from $r - p > r - q$ and $r - p \ne p$ (else $r = q$) we get $r - p = q = 2p$, so $r = 3p$; and $\gcd K = p = 1$. Hence $K = \{1, 2, 3\}$, and indeed $u_{\{1,2,3\}}(1/7) = (3/7)/(6/7) = 1/2 = 1/(d-1)$, so the configuration occurs. This proves (ii).

For $d=2$ the inequality $2d > d+2$ in Step 1 fails, and [2] exhibits $\mathrm{e}(F_2, \{a, a^2, b, b^2\}) = 5$; so the two values of d for which a diagonal realisation exists are exactly 2 and 3. $\square$

Remark 5.5. Theorem 5.4 rests on no computation, but two independent searches were run against it, in exact rational arithmetic and outside the formal development. Evaluating (6) over every K with $|K| \le 3$ and $\max K \le 45$: at $d=3$ the only K with $u_K(1/7) = 1/2$ is $\{1,2,3\}$, and at $d=4$ no K has $u_K(1/9) = 1/3$. Evaluating the criterion of Corollary 2.2 over all tuples $(K_1, \dots, K_d)$ with $\max K_i \le 18$ and $|K_i| \le 5$, for $2 \le d \le 12$: realisations of $2d+1$ occur only at $d=2$ and $d=3$. Lemma 5.1 itself was checked directly for every K with $\max K \le 14$, $|K| \le 4$ and $j \le 7$, with no violation.

Remark 5.6. At $d=2$ we make no classification claim. An exhaustive search over all pairs (K_1, K_2) with $\max K_i \le 20$ and $|K_i| \le 5$, evaluating the criterion of Corollary 2.2 in exact rational arithmetic, returns exactly three diagonal generating sets of F_2 with growth rate 5: the set $\{a, a^2, b, b^2\}$ of [2], and the two sets of Proposition 6.1. Whether the list is complete without the bounds $\max K_i \le 20$, $|K_i| \le 5$ we do not know.

Theorem 5.4 is proved by hand. Restricted to the interval sets, the same trichotomy is formalised, and it is the restriction that covers every example appearing in [2].

Theorem 5.7. *Let $d \ge 3$ and let $m_1, \dots, m_d$ be positive integers satisfying* (4). *Then there is an index i_0 with $m_i = 1$ for every $i \ne i_0$ and $2d = m_{i_0}(d-1)$; in particular $m_{i_0} \ne 1$, so exactly one entry differs from* 1. *For $d \ge 4$ equation* (4) *has no solution in positive integers at all, and so no diagonal generating set of F_d built from intervals has growth rate $2d+1$.*

Proof sketch. Let T be the set of indices with $m_i \ge 2$ and $j = |T|$. Bounding each term of (4) with $i \in T$ by $1/(d+2)$ and each term with $i \notin T$ by exactly $1/(d+1)$ gives

$$\frac{d-1}{d} \;\le\; \frac{j}{d+2} + \frac{d-j}{d+1} \;=\; \frac{d-1}{d} - \frac{jd-d-2}{d(d+1)(d+2)},$$

so $jd \le d+2$, forcing $j \le 1$ for $d \ge 3$. If $j=0$ then (4) reads $d/(d+1) = (d-1)/d$, i.e. $d^2 = d^2 - 1$, which is false. So $j=1$; writing i_0 for the single index in T and subtracting the $d-1$ terms equal to $1/(d+1)$ from both sides gives $1/(d+m_{i_0}) = (d-1)/\big(d(d+1)\big)$, i.e. $2d = m_{i_0}(d-1)$. For $d \ge 4$ this forces $m_{i_0} \le 2$ — since $m_{i_0} \ge 3$ would give $m_{i_0}(d-1) \ge 3d-3 > 2d$ — while $m_{i_0} \in \{1,2\}$ makes $2d = m_{i_0}(d-1)$ fail for $d \ge 4$; so no solution exists. The translation to generating sets is Corollary 2.2 together with (3), and is not part of the formal statement. $\square$

Theorem 5.8. *At $d=3$ the equation $\sum_{i=1}^{3} 1/(3+m_i) = 2/3$ has, in positive integers, exactly the solutions obtained from $(1,1,3)$ by permuting the entries. Under the translation of Corollary 2.2 this is the generating set $S_\star = \{a, b, c, c^2, c^3\}$, and $1/4 + 1/4 + 1/6 = 2/3$ confirms that it is a solution.*

Proof. By Theorem 5.7 a solution has exactly one entry $m_{i_0} \ne 1$, with $6 = 2d = m_{i_0}(d-1) = 2m_{i_0}$, so $m_{i_0} = 3$. $\square$

Uniqueness, and not merely existence, is what makes $S_\star$ canonical: among the interval sets, the $d=3$ answer is forced rather than chosen. Theorem 5.4(ii) extends this to arbitrary finite K_i, at the cost of leaving the formal development.

6. Two further realisations of 5, and controls

Proposition 6.1. *Besides $\{a, a^2, b, b^2\}$, the following diagonal generating sets of F_2 have growth rate* 5, *so that they too realise $5 \in \xi(F_2)$:*

$$\{a,\ b,\ b^2,\ b^3,\ b^4\} \qquad \text{and} \qquad \{a,\ b,\ b^3,\ b^8\}.$$

The first corresponds to the solution $(m_1, m_2) = (1,4)$ of (4) *at $d=2$; for the second, $K_2 = \{1,3,8\}$ is not an interval, and $u_{\{1,3,8\}}(1/5) = 1$ exactly.*

Proof. For the first set, $1/(2+1)+1/(2+4) = 1/3+1/6 = 1/2 = (d-1)/d$, so (4) holds at $d = 2$ and Corollary 2.2 applies. For the second, $\tau(\{1\}) = 2/3$ at $x_0 = 1/5$ and $\tau(\{1,3,8\}) = 1/(1+2\cdot 1) = 1/3$, and $2/3 + 1/3 = 1 = d-1$; the value $u_{\{1,3,8\}}(1/5) = 1$ is obtained by summing (1) in exact rational arithmetic, using that $\ell_{\{1,3,8\}}$ is eventually periodic with period $\max K = 8$ and slope 1. Only the first computation is part of the formal development. □

The second set matters because it shows the interval equation (4) does not see the whole solution set even at $d = 2$; that is why Theorem 5.4 needs Lemmas 5.1 and 5.3 rather than a computation with intervals.

We also record the negative controls, which exist to make the statements above falsifiable: they refute both a too-small and a too-large claim, and show the hypotheses are not vacuous.

Proposition 6.2. (i) Too small. *At radius* 3 *the ball of* F_3 *with respect to* $S_\star$ *has* 551 *elements and the ball with respect to a free basis has* 187*; and* $(m_1, m_2, m_3) = (1, 1, 1)$ *does not solve* (4) *at* $d = 3$*.*

(ii) Too large. *At radius* 3 *the ball with respect to* $\{a, a^2, b, b^2, c, c^2\}$ *has* 1093 *elements, against* 551*; and* $(2, 2, 2)$ *does not solve* (4) *at* $d = 3$*.*

(iii) Not vacuous. $S_\star$ *generates* F_3*; and at* $d = 4$ *the left-hand side of* (4) *does attain* $(d-1)/d$ *once the integrality of the* m_i *is dropped, since* $1/5 + 1/5 + 1/5 + 1/(4 + \frac{8}{3}) = 3/4$*. So the obstruction of Theorem 5.7 at* $d \geq 4$ *is integrality and not the equation itself.*

7. What remains open at $d \geq 4$

By Theorem 5.4(i), a generating set of F_d realising $2d+1$ for $d \geq 4$ cannot be diagonal: it must fail to respect any free-product decomposition of F_d into cyclic factors, and it has at least $d+2$ elements by Proposition 4.2. For such a set no product formula gives the growth series. The series is still rational — a hyperbolic group has only finitely many cone types with respect to any finite generating set, so its language of geodesics is regular and its growth series is a rational function; the cone-type argument goes back to Cannon [1], who established the corresponding linear recursion for the Cayley graphs of cocompact discrete hyperbolic groups — but obtaining the series requires building the cone-type (geodesic) automaton of the pair (F_d, S), which we have not done.

A numerical screen is not an alternative, and the reason is arithmetic rather than budget. The ratios $\sigma_S(n+1)/\sigma_S(n)$ converge to $\mathrm{e}(F_d, S)$ at the rate ρ^n, where ρ is the ratio of the second largest to the largest modulus among the reciprocals of the poles of $\Sigma_{F_d,S}$; for $S_\star$ those reciprocals are 7 and -3, so $\rho = 3/7$, and even there the ratio at radius 6 is still about 0.2 % away from 7 (the sphere sizes of Theorem 4.3 give $161250/23082 = 6.9860\ldots$). A candidate at $d = 4$ with ρ in the range 0.7–0.8, which nothing excludes, would need radius between about 16 and 26 before the ratios separate 9 from, say, 8.97; the corresponding balls have between $9^{16} \approx 2\cdot 10^{15}$ and $9^{26} \approx 6 \cdot 10^{24}$ elements. Only a method returning the exact rational series can decide such a case.

One remark narrows the search. Writing $w_i := 1 - 1/\Sigma_{G_i,S_i}(x_0)$ for the weight of a block in a free-product decomposition $F_d = G_1 * \cdots * G_r$ with $S = \bigsqcup_i S_i$, Proposition 2.1 turns the criterion into $\sum_i w_i = 1$. At $d = 4$, where $x_0 = 1/9$, a free cyclic block contributes $w = 1/5$, so the shortest route past Theorem 5.4 is one rank-2 block T together with two cyclic blocks, requiring $\Sigma_{F_2,T}(1/9) = 5/2$, that is $\sum_{g\neq 1} 9^{-|g|_T} = 3/2$. Writing $k = |T|$, the sphere sizes obey $\sigma_T(n) \leq 2k(2k-1)^{n-1}$, so for $k < 5$

$$\sum_{g\neq 1} 9^{-|g|_T} \;\leq\; \sum_{n\geq 1} \frac{2k(2k-1)^{n-1}}{9^{\,n}} \;=\; \frac{k}{5-k},$$

which is less than $3/2$ for $k \leq 2$ and equal to $3/2$ for $k = 3$ only if every inequality is an equality, that is only if T is a free basis of rank 3 — impossible inside F_2. In the other direction $\sigma_T(1) = 2k$ forces $2k/9 \leq 3/2$, so $k \leq 6$. Hence $|T| \in \{4, 5, 6\}$: the first case to examine is a rank-2 block with four, five or six generators.

8. Formal verification

The formal development is five modules in Lean 4 [7] on top of Mathlib [9]; there is no incomplete proof in it, and the axiom set of every headline declaration was printed. The dividing line is uniform: no statement of the form $\mathrm{e}(F_d, S) = \lambda$ is formalised, because every such statement passes through Proposition 2.1 and the free-product length formula behind it, which is not formalised — no proof-assistant library known to us carries growth series of groups in any form. What is formalised is everything on either side of that step. On the arithmetic side: Theorem 4.3(i)–(iii) in full, Theorem 5.7 and Theorem 5.8 in full, the equivalence $4d - 3 = 2d + 1 \Leftrightarrow d = 2$ and the geometric form $\sigma(n) = 4d\,(4d-3)^{n-1}$ of the model behind Proposition 3.4, the identity $1/3 + 1/6 = 1/2$ underlying the first set of Proposition 6.1, and both equation controls and the rational solution at $d = 4$ of Proposition 6.2. On the group side: the specification lemma identifying the enumerated finite sets with the word-metric balls, and the ball cardinalities of F_2 and F_3 at radii 0 to 3 for all four generating sets — Theorem 4.3(iv), Proposition 3.1, Proposition 3.4 and Proposition 6.2 — each matched term by term against the corresponding model, together with the finite set identities certifying that the generating sets are closed under inversion, and the fact that $S_\star$ generates F_3. Everything in the first list, together with the specification lemma and the generation of F_3 by $S_\star$, uses propositional extensionality, choice and quotient soundness only — this includes the limit of Theorem 4.3(iii) and the whole Diophantine classification; compiled evaluation is confined to the cardinality and finite-set statements, so every claim resting on exhaustive computation is one of those cardinalities, and the search in each case is the enumeration of the products of at most three generators of F_2 or F_3, the largest of them visiting 1093 reduced words. Not formalised, and stated as such where they appear, are Theorem 4.1, Proposition 4.2, Theorem 5.4, Proposition 2.1 with its corollary, the growth-rate values asserted in Propositions 3.1, 3.4 and 6.1, the second set of Proposition 6.1, and the searches reported in Remarks 3.3, 5.5 and 5.6, in the proof sketch of Theorem 4.3 and throughout Section 7. The repository is private; repository reference to be added at submission.

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