A MODEL SIFTING PROBLEM OF SELBERG

ZARATHUSTRA BRADY

Abstract. We study a model sifting problem introduced by Selberg, in which all of the primes have roughly the same size. We show that the Selberg lower bound sieve is asymptotically optimal in this setting, and we use this to give a new lower bound on the sifting limit β_κ in terms of the sifting dimension κ. We also show that one can use a rounding procedure to improve on the Selberg lower bound sieve by more than a constant amount in this setting, getting a lower order improvement which is asymptotic to the cube root of the main term.

1. Introduction

In a generic sifting problem, one has a (possibly weighted) set A (typically an interval) to be sifted, a set $\mathcal{P}$ of primes, and for each prime $p \in \mathcal{P}$ a number κ_p and a collection of κ_p distinct congruence classes $c_{p,1}, ..., c_{p,\kappa_p}$ modulo p to sift out. We define the sifted set $\mathcal{S}(A, \mathcal{P})$ (suppressing the dependence on the κ_ps and the choice of congruence classes $c_{p,i}$) to be

$$\mathcal{S}(A, \mathcal{P}) = \{a \in A \mid \forall p \in \mathcal{P}, a \not\equiv c_{p,1}, ..., c_{p,\kappa_p} \pmod{p}\}.$$

The goal is to find the best possible upper and lower bounds on the size of $\mathcal{S}(A, \mathcal{P})$, and especially to try to show that $\mathcal{S}(A, \mathcal{P})$ is nonempty.

We make the following additional definitions and assumptions. For squarefree d with all prime divisors coming from the set $\mathcal{P}$, we define a muliplicative function $\kappa(d)$ by

$$\kappa(d) = \prod_{p \mid d} \kappa_p,$$

and we define sets A_d by

$$A_d = \Big\{a \in A \mid \forall p \mid d, p \mid \prod_{i=1}^{\kappa_p}(a - c_{p,i})\Big\}.$$

We assume that there is a real number κ, called the *sifting dimension*, such that

$$\sum_{p \in \mathcal{P}} \frac{\log(p)}{p}\kappa_p = (\kappa + o(1)) \sum_{p \in \mathcal{P}} \frac{\log(p)}{p}.$$

We either make the strong assumption that

$$|A_d| = \frac{\kappa(d)}{d}|A| + O(\kappa(d))$$

or the weaker assumption

$$|A_d| = \frac{\kappa(d)}{d}|A|\Big(1 + O\Big(\frac{1}{\log(y/d)^{2\kappa+\epsilon}}\Big)\Big)$$

for some $\epsilon > 0$. As it turns out, which assumption we make has no effect on the main term of the final bounds one can obtain on the size of $|\mathcal{S}(A, \mathcal{P})|$, by Theorem 11 of [3].

We also define $y = |A|$, $z = \max \mathcal{P}$ (and typically $\mathcal{P}$ is the set of all primes below z), and a parameter s by $y = z^s$. Often one is interested in the case $A = [1, y]$ and $s = 2$, since a number $n \in [1, y]$ is prime if it has no prime factor smaller than $y^{1/2}$. We define a number β_κ, called the *sifting limit*, to be the infimum of values of s such that we can prove that $\mathcal{S}(A, \mathcal{P}) \neq \emptyset$ when $y = z^s$ becomes sufficiently large.

The method one uses to prove lower bounds on $|\mathcal{S}(A, \mathcal{P})|$ is to choose *sieve weights* λ_d such that

$$\mathcal{S}(A, \mathcal{P}) \geq \sum_d \lambda_d |A_d| \geq (1 + o(1))|A| \sum_d \frac{\kappa(d)}{d} \lambda_d.$$

In order to ensure the first inequality above, we need to choose the weights λ_d such that if we define $\theta(d)$ by

$$\theta(d) = \sum_{k|d} \lambda_k$$

then we have $\theta(1) \leq 1$ and $\theta(d) \leq 0$ for d having at least one prime divisor from the set $\mathcal{P}$. For the second inequality, we require λ_d to be 0 when $d > |A|$ (Lemma 2 of [3] shows that sieves which violate this assumption may always be replaced with sieves satisfying it, without affecting the main term of the bound on $\mathcal{S}(A, \mathcal{P})$).

In this paper, we will try to understand the asymptotics of the sifting limit β_κ as the sifting dimension κ goes to infinity, by studying a model sifting problem introduced by Selberg in Section 13 of [3], in which all of the primes have roughly the same size.

More precisely, let A be the interval $[1, y]$ and let $\mathcal{P}$ be a set of primes such that there is a number R with the property that the product of any R primes from $\mathcal{P}$ is below y, but the product of any $R + 1$ primes from $\mathcal{P}$ is greater than y (note that R is within 1 of the parameter s which appears in the usual sifting problem). Define a new parameter v, analogous to κ, by

$$v = \sum_{p \in \mathcal{P}} \frac{\kappa_p}{p}.$$

It isn't hard to see that the bounds we can get on $\mathcal{S}([1, y], \mathcal{P})$ only depend on the quantities v and R, since by an averaging argument we may assume without loss of generality that the sieve weights λ_d depend only on $\omega(d)$, the number of prime factors of d. For this reason we will switch the indices on our sieve weights from d to $\omega(d)$, so we need to optimize only $\lambda_0, ..., \lambda_R$, with $\lambda_0 = 1$. We make the definition

$$\theta(n) = \sum_{i=0}^{R} \lambda_i \binom{n}{i}.$$

Thus, the upper bound sieve reduces to trying to minimize the quantity

$$\sum_{n \geq 0} \frac{\theta(n)}{n!} v^n = e^v \sum_{n=0}^{R} \frac{\lambda_n}{n!} v^n$$

subject to the constraint $\theta(n) \geq 0$ for $n \in \mathbb{N}$. Similarly, the lower bound sieve reduces to trying to maximize the same quantity subject to the constraint $\theta(n) \leq 0$ for $n \in \mathbb{N}^+$. For every R, we let v_R be the largest v such that the optimal lower bound is nonnegative. Note that for the purpose of computing v_R, we can ignore the normalization $\lambda_0 = 1$.

Selberg [3] shows that $\lfloor \frac{R+1}{2} \rfloor \leq v_R \leq R$ (this is equation (13.22‴) of Section 13 of [3]), and that for any v, R the optimal θ takes the form

$$\theta(n) = \prod_i \left(1 - \frac{n}{\nu_i}\right)\left(1 - \frac{n}{\nu_i + 1}\right)$$

with $\nu_i \in \mathbb{N}$ for the upper bound sieve, and

$$\theta(n) = (1 - n) \prod_i \left(1 - \frac{n}{\nu_i}\right)\left(1 - \frac{n}{\nu_i + 1}\right)$$

with $\nu_i \in \mathbb{N}$ for the lower bound sieve (these are equations (13.6) and (13.6′) of Section 13 of [?]). Furthermore, Selberg [3] shows that each $\nu_i \leq \max(2R + 2v, R + 4v)$ (this is equation (13.8) of Section 13 of [3]), so for any v, R the optimal θ can be found with a finite amount of computation.

There are striking parallels between the model sifting problem and the usual sifting problem. For instance, consider the case where $v \leq 1$. In this case, we find that the optimal sieve has $\theta(n) = 0$ for $n = 1, ..., R$ or for $n = 1, ..., R-1$ (depending on whether it is an upper bound sieve or a lower bound sieve and on the parity of R), and the corresponding sieve weights are given by $\lambda_i = (-1)^i$ for $i \leq R$ or $i \leq R-1$ and $\lambda_i = 0$ otherwise (to see that this choice of $\theta(n)$ is optimal, we just have to check that the function $\theta(n)$ can't be improved by moving any single root when $v \leq 1$ - the details are left as an exercise to the reader). Correspondingly, it is conjectured that for $\kappa \leq 1$ the best upper and lower bound sieves are the β-sieves, which have $\lambda_d \in \{\mu(d), 0\}$ for all d.

More parallels are given in [3], where bounds on $\limsup \frac{R}{v_R}$ and $\limsup \frac{\beta_\kappa}{\kappa}$ are computed using various sieves. Using the combinatorial sieve, we get that $\limsup \frac{R}{v_R} \leq 3.591...$, where $3.591...$ is the solution to the exponential equation $e^{1+1/x} = x$ (see equation (13.19) of Section 13 of [3]). Precisely the same constant appears in the analysis of the β-sieve for the usual sifting problem: using the β-sieve, we can show that $\limsup \frac{\beta_\kappa}{\kappa} \leq 3.591...$ (this is equation (14.1) of [3]). Similarly, using the Selberg lower bound sieve it is shown in [3] (see equations (13.22′′) and (14.14) of [3]) that both $\limsup \frac{R}{v_R} \leq 2$ and $\limsup \frac{\beta_\kappa}{\kappa} \leq 2$. However, the analogy between the model problem and the usual sifting problem is not perfect: in the case of the model problem, an analogue of the Ankeny-Onishi sieve (described implicitly by equation (13.13) of [3]) gives the bound $\limsup \frac{R}{v_R} \leq 2.882...$, where $2.882...$ is the solution to the exponential equation $(\log(2)x+1)e^{1+1/x} = 4x$ (see the discussion after equation (13.20) of [3]), while the usual Ankeny-Onishi sieve gives $\limsup \frac{\beta_\kappa}{\kappa} \leq 2.445...$, where

$$2.445... = 2\exp\left(\int_0^{\log(2)} \frac{e^t - 1}{t} dt - 1 - \log\log(2)\right).$$

See the discussion around equation (14.12) of [3] (which cites [1] for the first computation of the above constant) for details.

The main result of this paper shows that $\lim \frac{R}{v_R} = 2$, and bounds the difference between v_R and $\lfloor \frac{R+1}{2} \rfloor$ between the square root and the cube root of R (up to constants). Based on the analogy outlined above, this may be regarded as weak evidence for $\lim \frac{\beta_\kappa}{\kappa} = 2$, and possibly also as weak evidence for $2\kappa - \beta_\kappa \gg \sqrt[3]{\kappa}$.

Theorem 1. *For $R = 2d+1$, we have $2\sqrt{d} \geq v_R - (d+1) \geq (c + o(1))\sqrt[3]{d}$, where $c \approx \frac{1}{12.14}$ is the positive solution of the equation*

$$\int_0^\infty \frac{1}{x^{3/2}} \min\left(\sin^2\left((\tfrac{x}{3} + c)\sqrt{x}\right), \cos^2\left((\tfrac{x}{3} + c)\sqrt{x}\right)\right) dx = 2\pi c.$$

From the upper bound on v_R we can deduce a lower bound on the usual sifting limit β_κ, improving Selberg's lower bound by a factor of 2.

Corollary 1. *If β_κ is the sifting limit of a sieve of dimension $\kappa \geq 3$, then*

$$\beta_\kappa > \frac{2\lfloor \kappa - \sqrt{\kappa} \rfloor + 1}{e^{1+\frac{1}{\sqrt{\kappa}}}}.$$

Proof. Suppose $\beta_\kappa < 2d+3$ for some $d \in \mathbb{N}$. For any y, let $\mathcal{P}$ be the set of primes between $y^{\frac{1}{2d+3}}$ and y^{1/β_κ}. Then if we take $v = \sum_{p \in \mathcal{P}} \frac{\kappa}{p}$, we see that

$$v = (\kappa + o(1)) \log\left(\frac{2d+3}{\beta_\kappa}\right).$$

Since the product of any $2d+3$ primes from $\mathcal{P}$ is greater than y, if we can find a nontrivial lower bound sieve then we must certainly have

$$\kappa \log\left(\frac{2d+3}{\beta_\kappa}\right) \le v_{2d+2} = v_{2d+1} \le d + 2\sqrt{d} + 1.$$

Rearranging, we find that

$$\beta_\kappa \ge \frac{2d+3}{e^{\frac{d+2\sqrt{d}+1}{\kappa}}}.$$

To finish, we take $d = \lfloor \kappa - \sqrt{\kappa} \rfloor - 1$. □

We prove the upper bound on v_R in Section 2. The main idea of the argument is to relax the problem by allowing $\theta(n)$ to be any polynomial of the form $(1-n)f(n)f(n-1)$ (f a degree d polynomial), without requiring that the roots of f be integers, and to note that any linear function of the coefficients of θ is a quadratic form in the coefficients of f.

In Section 3, we prove a result showing that when $v = v_R$, the optimal choice for θ does not have a root at 2. Based on the results of later sections, it appears that in the optimal lower bound sieve, the smallest roots of $\theta(n)$ are located at 1 and at $3, 4, 5, ..., \epsilon\sqrt[3]{d}$ for some $\epsilon > 0$.

In Section 4, we investigate the roots of the polynomial corresponding to Selberg's lower bound sieve. In Section 5, we finally prove the lower bound on v_R. The idea of the proof is to try to round each pair of repeated roots of the polynomial given by the Selberg lower bound sieve both up and down to the nearest integers. If we perform this rounding procedure directly, there is no guarantee that we actually improve on Selberg's sieve, so instead we do a sort of partial rounding: for each pair of repeated roots, we push the two roots away from each other (keeping their product fixed) until one of them becomes an integer.

2. Upper bound on v_R

Theorem 2. *Let $R = 2d+1$. Then $v_R \le d + 2\sqrt{d} + 1$.*

Proof. Assume that $d \ge 1$, since it is easy to check we have equality for $d = 0$. Since any optimal θ takes the form $(1-n)f(n)f(n-1)$ for some polynomial f of degree d, it's enough to show that for $v = d + 2\sqrt{d} + 1$ and any polynomial f of degree d we have

$$\sum_{n\ge 0} \frac{(1-n)f(n)f(n-1)}{n!} v^n \le 0.$$

Write

$$f(n) = \sum_{i=0}^{d} l_i \binom{n}{i}.$$

Define y_i, Δ_i, s_i by

$$y_r = (-1)^r \sum_{i\ge 0} \frac{l_{r+i}}{i!} v^i,$$

and $\Delta_r = y_r - y_{r+1}$, $s_r = \sum_{i\ge 0} y_{r+i}$. Using the identity

$$\binom{n}{a}\binom{n}{b} = \sum_k \frac{k!}{(k-a)!(k-b)!(a+b-k)!}\binom{n}{k},$$

we see that the variables y_r diagonalize the quadratic form corresponding to the Selberg upper bound sieve:

$$\sum_{n\ge 0} \frac{f(n)^2}{n!} v^n = e^v \sum_r \frac{y_r^2}{r!} v^r.$$

Since shifting the argument of f by ± 1 has the effect of replacing the y_rs with either the Δ_rs or the s_rs, we have

$$\sum_{n\geq 0}\frac{(1-n)f(n)f(n-1)}{n!}v^n = \sum_{n\geq 0}\frac{f(n)f(n-1)}{n!}v^n - v\sum_{n\geq 0}\frac{f(n+1)f(n)}{n!}v^n = e^v\sum_r \frac{v^r}{r!}y_r(s_r - v\Delta_r).$$

Dividing by e^v and rewriting this entirely in terms of the s_i, it becomes

$$\sum_r \frac{v^r}{r!}s_r(s_r - s_{r+1} - v(s_r - 2s_{r+1} + s_{r+2}) + r(s_{r-1} - 2s_r + s_{r+1})).$$

Comparing this to $\sum_r \frac{v^{r+1}}{r!}\Delta_r^2$, we get

$$\begin{aligned} &-2\sum_r \frac{v^r}{r!}s_r(s_r - s_{r+1} - v(s_r - 2s_{r+1} + s_{r+2}) + r(s_{r-1} - 2s_r + s_{r+1})) \\ &= \sum_r \frac{v^{r+1}}{r!}\Delta_r^2 + \sum_r \frac{v^r}{r!}\left((v-r-2)s_r^2 - 2(v-r-1)s_r s_{r+1} + (v-r)s_{r+1}^2\right). \end{aligned}$$

We just have to prove that the last sum above is nonnegative. Since $s_{d+1} = 0$, for any constant a we have

$$\begin{aligned} &\sum_r \frac{v^r}{r!}\left((v-r-2)s_r^2 - 2(v-r-1)s_r s_{r+1} + (v-r)s_{r+1}^2\right) \\ &= as_0^2 + \sum_r \frac{v^r}{r!}\left((v-r-2-a)s_r^2 - 2(v-r-1)s_r s_{r+1} + \left(v - r + a\frac{v}{r+1}\right)s_{r+1}^2\right). \end{aligned}$$

Thus it is enough to show that we can choose $0 \leq a \leq v - d - 2$ satisfying

$$(v-r-2-a)\left(v - r + a\frac{v}{r+1}\right) \geq (v-r-1)^2$$

for all $r < d$. It's easy to see that it is enough to check this for $r = d-1$, in which case it reduces to the inequality

$$(v-d)^2 a \geq va^2 + (v+d)a + d.$$

Taking $a = \sqrt{\frac{d}{v}}$ and $v = d + 2\sqrt{d} + 1$, we get equality. □

Remark 1. Numerical calculations indicate that for large d the quadratic form

$$\sum_r \frac{v^r}{r!}y_r(s_r - v\Delta_r)$$

is negative definite for $v \approx d + \frac{\sqrt{d}}{2} + 1$, so the above argument is probably not best possible.

Theorem 3. *For all d sufficiently large, if we take $v = d + \sqrt{\frac{d}{11}} + 1$,*

$$y_r = d + 1 - r - \frac{1}{\sqrt{2d}}\binom{d+2-r}{2},$$

and define $\Delta_r = y_r - y_{r+1}$, $s_r = \sum_{i=0}^{d-r} y_{r+i}$, then we have

$$\sum_{r=0}^{d}\frac{v^r}{r!}y_r(s_r - v\Delta_r) > 0.$$

Proof. Generally, if we let $k = v - (d+1)$ and take $y_r = d + 1 - r + a\binom{d+2-r}{2}$, then after a lengthy computation we find that

$$\sum_{r=0}^{d} \frac{v^r}{r!} y_r(s_r - v\Delta_r) = \left(\sum_{r=0}^{d} \frac{v^r}{r!}\right)\Bigg(-\frac{1}{2}k(d+k^2+1) - \frac{1}{12}\left(3(d+1)^2 - 6k^2(2d+1) - 5k^4 + 16k(d+1)\right) a$$
$$+ \frac{1}{12}\left(3k(d+1)^2 - k^3(4d-2) - k^5 + 2(d+1)^2 + 14k^2(d+1)\right) a^2 \Bigg)$$
$$+ \frac{v^{d+1}}{d!} \Bigg(\frac{1}{2}k(k-1) - \frac{1}{12}\left(7kd + 5k^2(k-1) - 3(d+1) + 11k\right) a$$
$$- \frac{1}{12}\left(d(4d+21) - k^2(3d-1) - k^4 + 13k(d+1) + k^3 - 13\right) a^2 \Bigg).$$

If k is within a constant factor of $\sqrt{d}$, we have the approximation

$$\frac{d!}{v^d} \sum_{r=0}^{d} \frac{v^r}{r!} = \Gamma(d+1, v) v^{-d} e^v = \operatorname{erfc}\left(\frac{k}{\sqrt{2d}}\right) e^{\frac{k^2}{2d}} \sqrt{\frac{\pi d}{2}} + O(1).$$

Plugging in $d = 11k^2$ and $a = -\frac{1}{k\sqrt{22}}$ and expanding everything to first order in k, we get the theorem. □

Remark 2. The preceding Theorem should be seen as a limitation of our method of producing upper bounds rather than an indication that $v_R - (d+1) \gg \sqrt{d}$. Numerical calculations show that the roots of the corresponding polynomial f are almost equal to the roots of the polynomial Selberg constructed to show $v_R \geq d+1$, except that the smallest root is approximately $\frac{5}{2}$ instead of being approximately 3. It appears that this change to the smallest root alone accounts for most of the improvement to v, and it is only permitted since we have relaxed the condition that $\theta(n) \leq 0$ for positive integers n to the much less restrictive condition that the roots of θ come in pairs that differ by at most 1.

It would be interesting to see if better upper bounds on v_R could be produced by incorporating the constraint that for every k the kth root of f is at least $2k+1$ (using the result of the next section).

3. 2 is not a root of the optimal θ

Theorem 4. *Let θ be the polynomial of degree R with $\theta(0) = 1$ and $\theta(n) \leq 0$ for all positive integers n. Suppose that $\theta(2) = 0$ and that*

$$\sum_n \frac{\theta(n)}{n!} v^n \geq 0.$$

Then there is another polynomial θ_2 of degree R with $\theta_2(0) = 1$, $\theta_2(n) \leq 0$ for all positive integers n, $\theta_2(2) < 0$, and

$$\sum_n \frac{\theta_2(n)}{n!} v^n > 0.$$

Proof. Assume without loss of generality that θ is of the form

$$\theta(n) = (1-n) \prod_i \left(1 - \frac{n}{\nu_i}\right)\left(1 - \frac{n}{\nu_i + 1}\right)$$

for ν_i positive integers with $\nu_1 = 2$, $\nu_{i+1} \geq \nu_i + 2$. Let $2k$ be the first integer which is not a root of θ (it is necessarily even). Define θ_2 by

$$\theta_2(n) = \frac{n-2k}{k(n-2)}\theta(n).$$

Then we have

$$\sum_n \frac{\theta_2(n)}{n!}v^n \geq 1 + \frac{\theta_2(2)}{2}v^2 + \frac{1}{k}\sum_{n>2k}\frac{\theta(n)}{n!}v^n \geq 1 + \frac{\theta_2(2)}{2}v^2 - \frac{1}{k}\left(1 + \frac{\theta(2k)}{(2k)!}v^{2k}\right).$$

We claim that

$$\frac{|\theta(2k)|}{(2k)!} > \left(\frac{|\theta_2(2)|}{2}\right)^k.$$

Since for any $\nu > 2k$ we have

$$1 - \frac{2k}{\nu} < \left(1 - \frac{2}{\nu}\right)^k,$$

we just need to show that

$$\left|1 - \frac{2k}{2}\right|\left|1 - \frac{2}{2k}\right|^{-k}\prod_{\nu\neq 2,2k}\left|1 - \frac{2k}{\nu}\right|\left|1 - \frac{2}{\nu}\right|^{-k} \geq \frac{(2k)!}{2^k},$$

but in fact the left hand side is a telescoping product which is precisely equal to the right hand side. Thus

$$1 + \frac{\theta_2(2)}{2}v^2 - \frac{1}{k}\left(1 + \frac{\theta(2k)}{(2k)!}v^{2k}\right) > 1 - \frac{|\theta_2(2)|}{2}v^2 - \frac{1}{k}\left(1 - \left(\frac{|\theta_2(2)|}{2}v^2\right)^k\right) > 0. \qquad \square$$

4. Properties of Selberg's construction

Let $R = 2d+1$. In order to show that $v_R \geq d+1$, Selberg [3] finds the optimal θ of the form

$$\theta(n) = (1-n)f(n)^2.$$

If we write

$$f(n) = \sum_i l_i \binom{n}{i},$$

and define y_i, Δ_i by

$$y_r = (-1)^r \sum_{i\geq 0}\frac{l_{r+i}}{i!}v^i,$$

and $\Delta_r = y_r - y_{r+1}$, then we find that

$$e^{-v}\sum_{n\geq 0}\frac{(1-n)f(n)^2}{n!}v^n = \sum_r \frac{v^r}{r!}y_r^2 - \sum_r \frac{v^{r+1}}{r!}\Delta_r^2.$$

Using Cauchy-Schwarz, Selberg [3] (see the discussion around equation (13.21) of [3]) shows that this is optimized when the Δ_rs are all equal, and in this case the above sum is nonnegative exactly for $v \leq d+1$.

Thus we substitute $y_r = d+1-r$, $v = d+1$, so

$$l_r = (-1)^r \sum_{i=0}^{d+1-r}\frac{d+1-r-i}{i!}(d+1)^i,$$

and we wish to describe the behavior of the roots $\nu_1, ..., \nu_d$ of $f(n) = \sum_i l_i\binom{n}{i}$ as d gets large.

Proposition 1. *The roots $\nu_1, ..., \nu_d$ of f are all real, positive, and greater than 2. For any integer n, the closed interval $[n, n+1]$ contains at most one root ν_i.*

Proof. These all follow from the optimality of $f(n)$ and simple smoothing arguments. $\square$

Corollary 2. *If n is an integer with $f(n)f(n+2) < 0$, then the interval $(n, n+2)$ contains exactly one root ν_i, and whether ν_i is above or below $n+1$ is determined by the sign of $f(n+1)$.*

From here on we assume that $\nu_1 < \cdots < \nu_d$.

Remark 3. Numerical calculations indicate that we even have $\nu_{i+1} > \nu_i + 2$ for every i.

Proposition 2. *Let n be a nonnegative integer. Then*

$$f(n+2) = \frac{(d+1)^{d+1}}{d!} \sum_k \frac{(-1)^k}{(d+1)^{k+1}} k! \binom{d}{k} \binom{n}{k}.$$

Furthermore, we have $f(0) = \frac{(d+1)^{d+1}}{d!}$.

Proof. Every time we shift the argument of f by 1, we replace the y_rs with their differences. Since the y_rs are linear, after shifting the argument of f twice all but the last of them is 0, which gives us

$$f(n+2) = \sum_k \frac{(-1)^k}{(d-k)!} (d+1)^{d-k} \binom{n}{k}.$$

Rearranging this, we get the first formula.

For the second formula, we have

$$f(0) = l_0 = \sum_{i=0}^{d} \frac{(d+1)^i}{i!}(d+1-i) = \sum_{i=0}^{d} \frac{(d+1)^{i+1}}{i!} - \frac{(d+1)^i}{(i-1)!} = \frac{(d+1)^{d+1}}{d!}.$$ $\square$

By the previous Proposition, the function

$$g(n) = \frac{d!}{(d+1)^{d+1}} f(n)$$

is normalized to have $g(0) = 1$.

Proposition 3. *Let $a(n,k)$ be the number of permutations of an n-set having exactly k cycles of size greater than 1. Then for n a nonnegative integer we have*

$$g(n+2) = \frac{1}{(d+1)^{n+1}} \sum_k (-1)^k a(n,k) d^k.$$

In particular, $g(n+2)$ is positive for large d if and only if $\lfloor \frac{n}{2} \rfloor$ is even.

More generally, define $a_q(n,k)$ by

$$a_q(n,k) = \sum_l \binom{n}{l} c_2(n-l,k) q^l,$$

where $c_2(m,k)$, an associated signless Stirling number of the first kind, is defined to be the number of derangements of an m-set having exactly k cycles of size greater than 1 (so that $a(n,k) = a_1(n,k)$ and $c_2(n,k) = a_0(n,k)$). Then we have

$$\sum_j (-1)^j (d+q)^{n-j} j! \binom{d}{j} \binom{n}{j} = \frac{n!}{2\pi i} \int_C e^{(d+q)z} (1-z)^d \frac{dz}{z^{n+1}} = \sum_k (-1)^k a_q(n,k) d^k,$$

where C is any contour winding counterclockwise around 0.

Proof. To prove the identity

$$\sum_j (-1)^j (d+q)^{n-j} j! \binom{d}{j}\binom{n}{j} = \frac{n!}{2\pi i}\int_C e^{(d+q)z}(1-z)^d \frac{dz}{z^{n+1}}$$

we just need to evaluate the nth derivative, with respect to z, of $e^{(d+q)z}(1-z)^d$ at $z=0$. Using the Leibniz rule we see that this is precisely the left hand side.

Now suppose that C is a circle of radius less than 1. Then we may use the power series for $\log(1-z)$ to see that

$$\begin{aligned} n! e^{(d+q)z}(1-z)^d &= n! \exp\left(qz - d\frac{z^2}{2} - d\frac{z^3}{3} - \cdots\right) \\ &= \sum_{l_1,l_2,\ldots\geq 0} z^{\sum_j j l_j} \frac{n!}{\prod_j j^{l_j} l_j!} q^{l_1}(-d)^{\sum_{j\geq 2} l_j}. \end{aligned}$$

Writing $l = l_1, k = \sum_{j\geq 2} l_j$, and interpreting l_j as the number of cycles of length j in a permutation, we see that the z^n-coefficient of this series is precisely

$$\sum_{k,l}\binom{n}{l} c_2(n-l,k) q^l (-d)^k = \sum_k (-1)^k a_q(n,k) d^k. \qquad \square$$

Corollary 3. *If k is fixed then ν_k approaches $2k+1$ from above as d goes to ∞.*

Proof. By the previous proposition, for any $m \geq 1$ we can find d_0 sufficiently large that for any $d \geq d_0$ we have $\nu_j \in (2j+1, 2j+2)$ for $1 \leq j \leq k+m^2$. For any $d \geq d_0$, we then have

$$\prod_{j\neq k}\left|\frac{\nu_j - (2k+1)}{\nu_j - (2k+2)}\right| \geq \prod_{1\leq j<k}\frac{2j-1}{2j}\prod_{1\leq j\leq m}\frac{2j+1}{2j} \gg_k \sqrt{m}.$$

By the previous proposition, we have

$$\prod_j \left|\frac{\nu_j - (2k+1)}{\nu_j - (2k+2)}\right| = \frac{|g(2k+1)|}{|g(2k+2)|} \to \frac{a(2k-1,k-1)}{a(2k,k)}$$

as $d \to \infty$, so we must have $\left|\frac{\nu_k - (2k+1)}{\nu_k - (2k+2)}\right| \ll_k \frac{1}{\sqrt{m}}$ for d sufficiently large. Taking m to infinity, we see that $\lim_{d\to\infty} \nu_k = 2k+1$. $\square$

Proposition 4. *The coefficients $a(n,k)$ are log-concave in k, that is,*

$$a(n,k)^2 \geq a(n,k-1)a(n,k+1).$$

More generally, for any $q \geq 0$ the coefficients $a_q(n,k)$ are log-concave in k.

Proof. This will be an application of Theorem 2.5.2 of Francesco Brenti's memoir on log concavity [2] (since the proof is short, we'll reproduce it here). We will show more generally that if q_i is a finite nonnegative log-concave sequence without internal zeros, then the expression

$$c_k = \sum_{m\geq 0}\frac{k!}{m!} c_2(m,k) q_m$$

is log-concave in k. Plugging in $q_m = m!\binom{n}{m}q^{n-m}$ gives (a stronger form of) the Proposition.

We start with the easy observation that for any i, j we have

$$\binom{i+j}{i} c_2(m, i+j) = \sum_{x+y=m}\binom{m}{x} c_2(x,i) c_2(y,j).$$

Thus, if we define the matrix L by $L_{k,m} = \frac{k!}{m!} c_2(m,k)$, then L has the "semigroup property" of Francesco Brenti [2], that is, the $i+j$th row of the matrix L is the convolution of the ith row and the jth row for any i, j.

The second ingredient we need is that every two by two minor of L is nonnegative. Since every entry of L is nonnegative, with $L_{k,n} = 0$ exactly when $2k > n$, this will follow from the inequality

$$c_2(n,k)c_2(n+1,k+1) \geq c_2(n,k+1)c_2(n+1,k). \tag{1}$$

Applying the recurrence

$$c_2(m,l) = (m-1)(c_2(m-1,l) + c_2(m-2,l-1))$$

with $(m,l) = (n+1,k+1), (n+1,k), (n,k)$, and $(n-1,k-1)$, we see that (1) is equivalent to

$$(n-1)(c_2(n-1,k)+c_2(n-2,k-1))c_2(n-1,k) \geq (n-2)c_2(n,k+1)(c_2(n-2,k-1)+c_2(n-3,k-2)),$$

which follows from the log-concavity of $c_2(m+l,l)$ in l for $m = n-k-1$ fixed. The log-concavity of $c_2(m+l,l)$ in l is well-known and can be proved by an easy induction on m using the above recurrence (in fact, by Theorem 6.7.2 of [2] $c_2(m+l,l)$ is even a Pólya frequency sequence in l).

Now we can apply the proof of Theorem 2.5.2 of [2]. Let Q be the matrix defined by $Q_{i,j} = q_{i+j}$, then if q_i is log-concave every two by two minor of Q will be nonpositive. By the Cauchy-Binet identity, we see that every two by two minor of

$$C = LQL^t$$

is nonpositive as well. We have

$$\begin{aligned} C_{i,j} &= \sum_{x,y} L_{i,x}Q_{x,y}L_{j,y} \\ &= \sum_m \left(\sum_{x+y=m} L_{i,x}L_{j,y} \right) q_m \\ &= \sum_m L_{i+j,m}q_m \\ &= c_{i+j}, \end{aligned}$$

so the nonpositivity of the two by two minors of C implies the log-concavity of c_k, and we are done. $\square$

Corollary 4. *If $\nu_k \geq 2k+2$, then*

$$4k^3 + 9k^2 - 4k \geq 9d.$$

Furthermore, for any fixed j, if k_j is the first integer k such that $\nu_k \geq 2k+1+j$ then as d goes to infinity we have

$$\lim_{d\to\infty} \frac{(2k_j)^3}{d} = \left(\frac{3\pi j}{2}\right)^2.$$

Proof. By the previous propositions, for the first claim it's enough to show that for $4k^3+9k^2-4k < 9d$ we have $a(2k,k)d > a(2k,k-1)$. We have

$$a(2k,k) = (2k-1)(2k-3)\cdots 1 = (2k-1)!!,$$

and

$$a(2k,k-1) = \binom{2k}{2}(2k-3)!!+2\cdot 2k\binom{2k-1}{3}(2k-5)!!+\frac{2^2}{2!}\binom{2k}{6}\binom{6}{3}(2k-7)!!+6\cdot\binom{2k}{4}(2k-5)!!,$$

so

$$\frac{a(2k,k-1)}{a(2k,k)} = k + \frac{4k(k-1)}{3} + \frac{4k(k-1)(k-2)}{9} + k(k-1) = \frac{4k^3+9k^2-4k}{9}.$$

For the second claim, we will apply Corollary 2 by showing that for every $k \ll \sqrt[3]{d}$, we have at least one of $g(k-1)g(k+1) < 0$ or $g(k)g(k+2) < 0$, depending on whether k is even or odd and on the size of $\sqrt{\frac{(2k)^3}{9d}}$ modulo 2π. More precisely, we will show that for $L \geq \frac{k^3}{d}$, we have

$$(-1)^k \frac{(d+1)^{2k+1}}{d^k a(2k,k)} g(2k+2) = \sum_l \frac{(-1)^l}{d^l} \frac{a(2k,k-l)}{a(2k,k)} = \cos\left(\sqrt{\tfrac{(2k)^3}{9d}}\right) + O_L(\tfrac{1}{k}) + O(\tfrac{1}{L!})$$

and

$$(-1)^k \frac{(d+1)^{2k+2}}{d^k a(2k+1,k)} g(2k+3) = \sum_l \frac{(-1)^l}{d^l} \frac{a(2k+1,k-l)}{a(2k+1,k)} = \sqrt{\tfrac{9d}{(2k)^3}} \sin\left(\sqrt{\tfrac{(2k)^3}{9d}}\right) + O_L(\tfrac{1}{k}) + O(\tfrac{1}{L!}).$$

In order to determine the size of $a(2k,k)$, we note that for any fixed l and k large, the largest contribution of permutations on $2k$ symbols with $k-l$ nontrivial cycles comes from the permutations with as few 2-cycles as possible, so we have

$$\frac{a(2k,k-l)}{a(2k,k)} = \frac{2^{2l}}{(2l)!}\binom{2k}{6l}\binom{6l}{3,\ldots,3}\frac{(2k-6l-1)!!}{(2k-1)!!} + O_l(k^{3l-1}) = \frac{(2k)^{3l}}{(2l)!3^{2l}} + O_l(k^{3l-1}).$$

Using the log-concavity of the $a(n,k)$s, we see that if we take L even and large enough that $a(2k,k-L)/d^L > a(2k,k-(L+1))/d^{L+1}$, then we have

$$\sum_{l \leq L+1} \frac{(-1)^l}{(2l)!}\left(\frac{(2k)^3}{9d}\right)^l + O_L\left(\frac{k^{3L+2}}{d^{L+1}}\right) \leq \sum_l \frac{(-1)^l}{d^l}\frac{a(2k,k-l)}{a(2k,k)} \leq \sum_{l \leq L} \frac{(-1)^l}{(2l)!}\left(\frac{(2k)^3}{9d}\right)^l + O_L\left(\frac{k^{3L-1}}{d^L}\right).$$

Taking $L \geq \frac{(2k)^3}{9d}$, we get

$$\sum_l \frac{(-1)^l}{d^l}\frac{a(2k,k-l)}{a(2k,k)} = \cos\left(\sqrt{\tfrac{(2k)^3}{9d}}\right) + O_L(\tfrac{1}{k}) + O(\tfrac{1}{L!}).$$

Similarly, for large k we have

$$\frac{a(2k+1,k-l)}{a(2k+1,k)} = \frac{(2k)^{3l}}{(2l+1)!3^{2l}} + O_l(k^{3l-1}),$$

which gives

$$\sum_l \frac{(-1)^l}{d^l}\frac{a(2k+1,k-l)}{a(2k+1,k)} = \sqrt{\tfrac{9d}{(2k)^3}} \sin\left(\sqrt{\tfrac{(2k)^3}{9d}}\right) + O_L(\tfrac{1}{k}) + O(\tfrac{1}{L!}).$$

Taking L sufficiently large, we see that for $k^3 \leq Ld$ (and k,d large) the sign of $g(k)g(k+2)$ is negative unless either k is even and $\sqrt{\frac{(2k)^3}{9d}}$ is close to a multiple of π, or k is odd and $\sqrt{\frac{(2k)^3}{9d}}$ is close to an odd multiple of $\frac{\pi}{2}$. Using Corollary 2, we see that

$$\lim_{d\to\infty} \frac{(2k_{2j-1})^3}{9d} = \left(\pi j - \frac{\pi}{2}\right)^2$$

and

$$\lim_{d\to\infty} \frac{(2k_{2j})^3}{9d} = (\pi j)^2. \qquad \square$$

Remark 4. Numerical calculations support the approximation

$$\nu_k \approx 2k+1+\frac{2}{3\pi}\sqrt{\frac{\nu_k^3}{d}}$$

when k is small compared to d. When $d=1000$ and $k\le 100$, the absolute error is less than 0.05. On the other hand, we seem to have $\nu_d \approx 4d$, so the approximation breaks down for large k.

Proposition 5. *Let*

$$\theta(n)=(1-n)g(n)^2.$$

For $(2k+2)^3\le 18\alpha d$, $\alpha\le 1$, *we have*

$$\frac{|\theta(2k+2)|}{(2k+2)!}(d+1)^{2k+2}\ge (1-\alpha)^2\frac{d^{2k}}{(d+1)^{2k}}\frac{1}{2}\frac{C_k}{4^k},$$

where $C_k=\frac{1}{k+1}\binom{2k}{k}$ *is the* k*th Catalan number, and*

$$\frac{|\theta(2k+1)|}{(2k+1)!}(d+1)^{2k+1}\ge\left(1-\frac{\alpha}{3}\right)^2\frac{d^{2k-2}}{(d+1)^{2k-2}}\frac{2k(k+1)(2k+1)}{9(d+1)}\frac{C_k}{4^k}.$$

Proof. By the log-concavity of the $a(n,k)$s, since $4k^3+9k^2-4k\le\frac{1}{2}(2k+2)^3\le 9\alpha d$ we have

$$|g(2k+2)|\ge\frac{d^k}{(d+1)^{2k+1}}\left(a(2k,k)-\frac{1}{d}a(2k,k-1)\right)\ge(1-\alpha)\frac{(2k-1)!!d^k}{(d+1)^{2k+1}},$$

so

$$\frac{|\theta(2k+2)|}{(2k+2)!}(d+1)^{2k+2}\ge(1-\alpha)^2\frac{d^{2k}}{(d+1)^{2k}}\frac{(2k+1)((2k-1)!!)^2}{(2k+2)!}=(1-\alpha)^2\frac{d^{2k}}{(d+1)^{2k}}\frac{1}{2}\frac{C_k}{4^k}.$$

Similarly, using the formulas

$$a(2k-1,k-1)=(2k-1)!!+2!\binom{2k-1}{3}(2k-5)!!=\frac{(2k+1)!!}{3}$$

and

$$\begin{aligned}a(2k-1,k-2)={}&\binom{2k-1}{3}(2k-5)!!+2!\binom{2k-1}{3}\binom{2k-4}{2}(2k-7)!!\\&+3!\binom{2k-1}{4}(2k-5)!!+4!\binom{2k-1}{5}(2k-7)!!\\&+\frac{2!^2}{2!}\binom{2k-1}{6}\binom{6}{3}(2k-7)!!+2!3!\binom{2k-1}{3}\binom{2k-4}{4}(2k-9)!!\\&+\frac{2!^3}{3!}\binom{2k-1}{9}\binom{9}{3,3,3}(2k-11)!!\\={}&\frac{(k-1)(20k^2+35k-123)}{405}(2k+1)!!,\end{aligned}$$

we see that since $(k-1)(20k^2+35k-123)\le\frac{5}{2}(2k+2)^3\le 135\frac{\alpha}{3}d$, we have

$$|g(2k+1)|\ge\frac{d^{k-1}}{(d+1)^{2k}}\left(a(2k-1,k-1)-\frac{1}{d}a(2k-1,k-2)\right)\ge\left(1-\frac{\alpha}{3}\right)\frac{(2k+1)!!d^{k-1}}{3(d+1)^{2k}},$$

so

$$\frac{|\theta(2k+1)|}{(2k+1)!}(d+1)^{2k+1}\ge\left(1-\frac{\alpha}{3}\right)^2\frac{d^{2k-2}}{(d+1)^{2k-2}}\frac{2k((2k+1)!!)^2}{9(d+1)(2k+1)!}=\left(1-\frac{\alpha}{3}\right)^2\frac{d^{2k-2}}{(d+1)^{2k-2}}\frac{2k(k+1)(2k+1)}{9(d+1)}\frac{C_k}{4^k}.$$

□

We can now give our first improvement on Selberg's lower bound sieve.

Theorem 5. *For every $d \geq 4$ there is a polynomial θ_d of degree $2d+1$ with $\theta_d(0) = 1$, $\theta_d(n) \leq 0$ for $n \in \mathbb{N}^+$, and*

$$\sum_n \frac{\theta_d(n)}{n!}(d+1)^n \gg \frac{1}{\sqrt[6]{d}}.$$

Proof. It's easy to see that for any root ν_k of g, we can find a quadratic polynomial q_k such that $q_k(0) = 1$,

$$0 \leq q_k(n) \leq \left(1 - \frac{n}{\nu_k}\right)^2$$

for $n \in \mathbb{N}$, and at least one of $q_k(\lfloor \nu_k \rfloor), q_k(\lceil \nu_k \rceil)$ is 0: for instance, we can take

$$q_k(n) = \left(1 - \frac{n}{\nu_k}\right)^2 - \min\left(\frac{1}{\lfloor \nu_k \rfloor}\left(1 - \frac{\lfloor \nu_k \rfloor}{\nu_k}\right)^2, \frac{1}{\lceil \nu_k \rceil}\left(1 - \frac{\lceil \nu_k \rceil}{\nu_k}\right)^2\right) n.$$

We define θ_d by

$$\theta_d(n) = (1-n)\prod_k q_k(n).$$

If we set $\theta(n) = (1-n)g(n)^2$, then we have

$$\sum_n \frac{\theta_d(n)}{n!}(d+1)^n \geq \sum_n \frac{\theta(n)}{n!}(d+1)^n + \sum_k \min\left(\frac{|\theta(\lfloor \nu_k \rfloor)|}{\lfloor \nu_k \rfloor !}(d+1)^{\lfloor \nu_k \rfloor}, \frac{|\theta(\lceil \nu_k \rceil)|}{\lceil \nu_k \rceil !}(d+1)^{\lceil \nu_k \rceil}\right).$$

Since $\sum_n \frac{\theta(n)}{n!}(d+1)^n = 0$ and $2k+1 \leq \nu_k \leq 2k+2$ for $(2k+2)^3 \leq 18d$, we can apply the previous Proposition to see that

$$\sum_n \frac{\theta_d(n)}{n!}(d+1)^n \geq \sum_{(2k+2)^3 \leq 18d} \left(1 - \frac{(2k+2)^3}{18d}\right)^2 \frac{d^{2k}}{(d+1)^{2k}} \min\left(\frac{1}{2}, \frac{2k(k+1)(2k+1)}{9(d+1)}\right) \frac{C_k}{4^k} \gg \frac{1}{\sqrt[6]{d}}.$$

□

5. Lower bound on v_R

We come at last to trying to prove a lower bound on v_R. For any $v \geq d+1$, we define the polynomial g_v by

$$g_v(n) = \frac{d!}{v^{d+1}} \sum_r l_r \binom{n}{r},$$

where

$$l_r = (-1)^r \sum_{k=0}^{d+1-r} \frac{d+1-r-k}{k!} v^k,$$

as in Selberg's construction.

Proposition 6. *For $q = v - d \ll \sqrt{d}$, we have*

$$g_v(0) = 1 - \frac{q-1}{v}\frac{d!}{v^d}\sum_r \frac{v^r}{r!} = 1 - \frac{q-1}{v}\Gamma(d+1, v)v^{-d}e^v \gg 1$$

as well as

$$\sum_n \frac{(1-n)g_v(n)^2}{n!} v^n = -e^v \frac{d!}{v^{d+1}}(q-1)g_v(0) = -(\sqrt{2\pi} + o(1))e^{\frac{q^2}{2d}} \frac{q-1}{\sqrt{d}} g_v(0).$$

Furthermore, for every nonnegative integer n we have

$$\frac{d}{dv}\left(v^{n+1}g_v(n+2)\right) = nv^n g_v(n+1)$$

and

$$g_v(n+2) = \frac{1}{v^{n+1}}\sum_k (-1)^k a_q(n,k)d^k.$$

Proof. The first two claims are easy calculations. For the last two claims, we use an analogous argument to the proof of Proposition 2 to see that

$$g_v(n+2) = \frac{1}{v^{n+1}}\sum_j (-1)^j v^{n-j} j! \binom{d}{j}\binom{n}{j}.$$

Multiplying by v^{n+1} and differentiating each term of the sum with respect to v we get the claim about the derivative of $v^{n+1}g_v(n+2)$. The last claim follows from Proposition 3. $\square$

Lemma 1. *For $0 \le k = v - d - 1 \le \frac{\sqrt[3]{d}}{3}$ and $1 \le j \le \sqrt[3]{d} - 1$ we have*

$$d^{j-1}\left(\frac{2j+1}{3} + k\right)(2j-1)!! \ge (-1)^{j-1}v^{2j}g_v(2j+1) \ge \left(1 - \frac{4}{27}\right)d^{j-1}\frac{(2j+1)!!}{3}$$

and

$$d^j(2j-1)!! \ge (-1)^j v^{2j+1}g_v(2j+2) \ge d^{j-1}\left(\frac{5d}{9} - \frac{2kj(2j+1)}{3} - k^2 j\right)(2j-1)!! \ge 0.$$

Proof. We prove these inequalities by induction on j. For the base case we use the identity $vg_v(2) = 1$. By the previous Proposition, we have

$$v^{2j}g_v(2j+1) = (d+1)^{2j}g(2j+1) + (2j-1)\int_{u=d+1}^{v} u^{2j-1}g_u(2j)du.$$

By the induction hypothesis, we have $(-1)^{j-1}g_u(2j) \ge 0$ and $(-1)^{j-1}u^{2j-1}g_u(2j) \le d^{j-1}(2j-3)!!$, so the claim follows from the bounds established on $g(2j+1)$ in Proposition 5. The second bound is proved the same way, except this time $(-1)^j v^{2j+1}g_v(2j+2)$ is decreasing in v. $\square$

Theorem 6. *If $R = 2d+1$ and $d \ge 8$ then $v_R - (d+1) \gg \sqrt[3]{d}$.*

Proof. By the same argument as the one used in the proof of Theorem 5, for any $v \le d + 1 + \frac{\sqrt[3]{d}}{3}$ we can find a polynomial θ_v of degree $2d+1$ with $\theta_v(0) = g_v(0)^2$,

$$0 \ge \theta_v(n) \ge (1-n)g_v(n)^2$$

for $n \in \mathbb{N}^+$, and such that for any $1 \le j \le \sqrt[3]{d} - 1$ at least one of $\theta_v(2j+1), \theta_v(2j+2)$ vanishes. Setting $k = v - d - 1$, we see that

$$\sum_n \frac{\theta_v(n)}{n!}v^n \ge \sum_n \frac{(1-n)g_v(n)^2}{n!}v^n + \sum_{1\le j\le \sqrt[3]{d}-1} \min\left(\frac{2jg_v(2j+1)^2}{(2j+1)!}v^{2j+1}, \frac{(2j+1)g_v(2j+2)^2}{(2j+2)!}v^{2j+2}\right).$$

By the previous Lemma and Proposition, this is at least

$$-e^v\frac{d!}{v^{d+1}}k + \sum_{1\le j\le \sqrt[3]{d}-1} \min\left(\left(1-\frac{4}{27}\right)^2\frac{2j(j+1)(2j+1)d^{2j-2}}{9v^{2j-1}},\right.$$

$$\left.\frac{1}{2}\left(\frac{5d}{9} - \frac{2kj(2j+1)}{3} - k^2 j\right)^2\frac{d^{2j-2}}{v^{2j}}\right)\frac{C_j}{4^j}.$$

The sum in the above is easily seen to be $\gg \frac{1}{\sqrt[6]{d}}$, and $e^v \frac{d!}{v^{d+1}} k \ll \frac{k}{\sqrt{d}}$, so for $k \ll \sqrt[3]{d}$ the above is positive. $\square$

The implied constant in the previous Theorem is very small. In order to get a better constant, we have to get more accurate bounds for g_v, and further we need the bounds to be valid in a larger range for j, k. One can argue similarly to Corollary 4 to show that if $j, k, d \to \infty$ with $j^3, k^3 \ll d$, and $v = d + k + 1$, then we have

$$(-1)^{j-1} v^{2j} g_v(2j+1) \approx d^{j-1} \sqrt{\tfrac{d}{2j}} \sin\left(\left(\tfrac{2j}{3} + k\right)\sqrt{\tfrac{2j}{d}}\right)(2j-1)!!$$

and

$$(-1)^j v^{2j+1} g_v(2j+2) \approx d^j \cos\left(\left(\tfrac{2j}{3} + k\right)\sqrt{\tfrac{2j}{d}}\right)(2j-1)!!,$$

but instead we will use the saddle point method to get a more accurate approximation.

Theorem 7. *If $n, q, d \geq 1$ with $4(n+q)^2 \leq d$, and if $v = d + q$, then we have*

$$v^{(n+2)/2} g_v(n+2) = \frac{n! e^{n/2}}{\sqrt{\pi} n^{(n+1)/2}} \Re\left(i^{-n} \exp\left(i(\tfrac{n}{3} + q)\sqrt{\tfrac{n}{v}} + O(\tfrac{n+q}{\sqrt{nv}})\right)\right) e^{\frac{q^2}{4v}}.$$

Proof. We compute $g_v(n+2)$ by the formula

$$v^{n+1} g_v(n+2) = \frac{n!}{2\pi i} \int_C e^{vz}(1-z)^d z^{-n} \frac{\mathrm{d}z}{z},$$

where the contour is taken to be a circle of radius $\sqrt{\frac{n}{v}}$ centered at the origin. Since the logarithmic derivative of the integrand is $v - \frac{d}{1-z} - \frac{n}{z}$, the integrand has saddle points at $z_0, \bar{z}_0$, where z_0 is the root of $vz_0^2 - (n+q)z_0 + n = 0$ having positive imaginary part.

Writing $z = \sqrt{\frac{n}{v}} e^{i\theta}$, $z_0 = \sqrt{\frac{n}{v}} e^{i\theta_0}$, we have

$$v^{(n+2)/2} g_v(n+2) = \frac{n!}{2\pi n^{n/2}} \int_0^{2\pi} e^{vz - in\theta}(1-z)^d \mathrm{d}\theta.$$

To see that we may restrict the integral to a small interval around θ_0 and $2\pi - \theta_0$, we consider the real part of the logarithm of the integrand as a function of $\cos(\theta)$:

$$\log|e^{vz-in\theta}(1-z)^d| = \sqrt{nv}\cos(\theta) + d\log\left|1 - \sqrt{\tfrac{n}{v}} e^{i\theta}\right| = \sqrt{nv}\cos(\theta) + \frac{d}{2}\log\left(1 + \frac{n}{v} - 2\sqrt{\tfrac{n}{v}}\cos(\theta)\right).$$

Taking the second derivative with respect to $\cos(\theta)$, we obtain

$$\frac{\mathrm{d}^2}{(\mathrm{d}\cos(\theta))^2} \log|e^{vz-in\theta}(1-z)^d| = -\frac{2dn}{v\left(1 + \frac{n}{v} - 2\sqrt{\frac{n}{v}}\cos(\theta)\right)^2} \leq -\frac{2dnv}{(\sqrt{v} + \sqrt{n})^4},$$

so

$$|e^{vz}(1-z)^d| \leq |e^{vz_0}(1-z_0)^d| e^{-\frac{dv}{(\sqrt{v}+\sqrt{n})^4} n(\cos(\theta) - \cos(\theta_0))^2},$$

and we see that we may restrict our attention to θ with $|\cos(\theta) - \cos(\theta_0)| \ll \frac{\log(n)}{\sqrt{n}}$. Since $\cos(\theta_0) = \frac{n+q}{2\sqrt{nv}} \leq \frac{1}{4}$, this is equivalent to restricting to the ranges $|\theta - \theta_0| \ll \frac{\log(n)}{\sqrt{n}}$ and $|\theta - (2\pi - \theta_0)| \ll \frac{\log(n)}{\sqrt{n}}$.

Around θ_0, the integrand can be written as

$$e^{vz_0 - in\theta_0}(1-z_0)^d \exp\left(\alpha(\theta - \theta_0)^2 + \beta(\theta - \theta_0)^3 + O(n(\theta - \theta_0)^4)\right),$$

with

$$\alpha = -\frac{vz_0}{2} + \frac{dz_0}{2(1-z_0)} + \frac{dz_0^2}{2(1-z_0)^2} = -n + \frac{(q-n)(vz_0-n)}{2d} = -n + O\Big((n+q)\sqrt{\tfrac{n}{v}}\Big),$$

$$\beta = -\frac{ivz_0}{6} + \frac{idz_0}{6(1-z_0)} + \frac{idz_0^2}{2(1-z_0)^2} + \frac{idz_0^3}{3(1-z_0)^3} = -\frac{2in}{3} + O\Big((n+q)\sqrt{\tfrac{n}{v}}\Big).$$

Thus we have

$$\exp\left(\alpha(\theta-\theta_0)^2 + \beta(\theta-\theta_0)^3 + O(n(\theta-\theta_0)^4)\right) = e^{\alpha(\theta-\theta_0)^2}(1+\beta(\theta-\theta_0)^3+O(n(\theta-\theta_0)^4+n^2(\theta-\theta_0)^6)),$$

and after integrating we get

$$\int_0^{2\pi} e^{vz-in\theta}(1-z)^d \mathrm{d}\theta = 2\Re\left(e^{vz_0-in\theta_0}(1-z_0)^d \tfrac{\sqrt{\pi}}{\sqrt{n}}(1+O(\tfrac{n+q}{\sqrt{nv}}))\right).$$

By the defining equation for z_0 we have $\frac{v}{n}z_0^2 = -1 + \frac{n+q}{n}z_0$, so

$$e^{-in\theta_0} = i^{-n}\left(1 - \frac{n+q}{n}z_0\right)^{-n/2} = i^{-n}\exp\left(\frac{n+q}{2}z_0 - \frac{(n+q)^2}{4v} + O(\tfrac{n+q}{\sqrt{nv}})\right).$$

Also, we have

$$e^{vz_0}(1-z_0)^d = \exp\left(\frac{n}{2} + \left(\frac{n}{3} + q - \frac{n+q}{2}\right)z_0 + \frac{n(n-2q)}{12v} + O(\tfrac{n+q}{\sqrt{nv}})\right),$$

so, using $z_0 = i\sqrt{\frac{n}{v}} + \frac{n+q}{2v} + O(\frac{(n+q)^2}{v^2})$, we have

$$v^{(n+2)/2}g_v(n+2) = \frac{n!}{\sqrt{\pi}n^{(n+1)/2}}\Re\left(i^{-n}\exp\left(\tfrac{n}{2} + i(\tfrac{n}{3}+q)\sqrt{\tfrac{n}{v}} + \tfrac{q^2}{4v} + O(\tfrac{n+q}{\sqrt{nv}})\right)\right). \qquad \square$$

Theorem 8. *If $R = 2d+1$ then $v_R - d \geq (c+o(1))\sqrt[3]{d}$, where $c \approx \frac{1}{12.14}$ is the positive solution of the equation*

$$\int_0^\infty \frac{1}{x^{3/2}}\min\left(\sin^2\left((\tfrac{x}{3}+c)\sqrt{x}\right), \cos^2\left((\tfrac{x}{3}+c)\sqrt{x}\right)\right)dx = 2\pi c.$$

Proof. Set $v = d+q$ with $q = (c+o(1))\sqrt[3]{d}$, and let ν_j be the jth root of g_v. Let $G_v(n)$ be defined by

$$G_v(n) = \frac{(n-1)g_v(n)^2}{n!}v^n.$$

Arguing as in Theorem 6, we just need to check that

$$\sum_n \frac{(1-n)g_v(n)^2}{n!}v^n + \sum_{j \ll \sqrt{v}} \min\left(G_v(\lfloor \nu_j \rfloor), G_v(\lceil \nu_j \rceil)\right) \geq 0.$$

As in Corollary 4, we have $\nu_j \approx 2j+1$, and applying the previous Theorem we get

$$\min\left(G_v(\lfloor \nu_j \rfloor), G_v(\lceil \nu_j \rceil)\right) \approx \frac{e^{\frac{q^2}{2v}}}{2\sqrt{\pi j^3}}\min\left(\sin^2\left((\tfrac{2j}{3}+q)\sqrt{\tfrac{2j}{v}}\right), \cos^2\left((\tfrac{2j}{3}+q)\sqrt{\tfrac{2j}{v}}\right)\right),$$

while from Proposition 6 we have

$$\sum_n \frac{(1-n)g_v(n)^2}{n!}v^n \approx -\sqrt{2\pi}e^{\frac{q^2}{2v}}\frac{q}{\sqrt{v}}.$$

Thus, we just need

$$\sum_{j \geq 1} \frac{1}{2\sqrt{\pi j^3}}\min\left(\sin^2\left((\tfrac{2j}{3}+q)\sqrt{\tfrac{2j}{v}}\right), \cos^2\left((\tfrac{2j}{3}+q)\sqrt{\tfrac{2j}{v}}\right)\right) \gtrsim \sqrt{2\pi}\frac{q}{\sqrt{v}}.$$

Writing $2j = x\sqrt[3]{v}, q = c\sqrt[3]{v}$ and approximating the sum by an integral, this becomes

$$\int_0^\infty \frac{1}{x^{3/2}} \min\left(\sin^2\left((\tfrac{x}{3}+c)\sqrt{x}\right), \cos^2\left((\tfrac{x}{3}+c)\sqrt{x}\right)\right) \mathrm{d}x \geq 2\pi c. \qquad \square$$

References

[1] N. C. Ankeny. Applications of the sieve. In *Proc. Sympos. Pure Math., Vol. VIII*, pages 113–118. Amer. Math. Soc., Providence, R.I., 1965.

[2] F. Brenti. *Unimodal, Log-concave and Pólya Frequency Sequences in Combinatorics*. Number no. 413 in Memoirs of the AMS Series. American Mathematical Soc.

[3] Atle Selberg. *Collected papers. Vol. II*. Springer-Verlag, Berlin, 1991. With a foreword by K. Chandrasekharan.

Department of Mathematics, Stanford University, 450 Serra Mall, Bldg. 380, Stanford, CA 94305-2125

E-mail address: `notzeb@stanford.edu`