On the first occurrences of gaps between primes in a residue class

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To the memory of Professor Thomas R. Nicely (1943–2019)

Abstract

We study the first occurrences of gaps between primes in the arithmetic progression

$$\text{(P)} \quad r,\ r+q,\ r+2q,\ r+3q,\ldots,$$

where q and r are coprime integers, $q > r \geq 1$. The growth trend and distribution of the first-occurrence gap sizes are similar to those of *maximal* gaps between primes in (P). The histograms of first-occurrence gap sizes, after appropriate rescaling, are well approximated by the Gumbel extreme value distribution. Computations suggest that first-occurrence gaps are much more numerous than maximal gaps: there are $O(\log^2 x)$ first-occurrence gaps between primes in (P) below x, while the number of maximal gaps is only $O(\log x)$. We explore the connection between the asymptotic density of gaps of a given size and the corresponding generalization of Brun's constant. For the first occurrence of gap d in (P), we expect the end-of-gap prime $p \asymp \sqrt{d}\exp(\sqrt{d/\varphi(q)})$ infinitely often. Finally, we study the gap size as a function of its index in the sequence of first-occurrence gaps.

1 Introduction

Let p_n denote the n-th prime number, and consider the difference between successive primes, called a *prime gap*: $p_{n+1} - p_n$. If a prime gap is *larger* than all gaps before it, we call this gap *maximal*. If a prime gap is either *larger* or *smaller* than every gap before it, we call this gap a *first occurrence*.

Denote by $G(x)$ the maximal gap between primes $\le x$:

$$G(x) \;=\; \max_{p_{n+1}\le x} (p_{n+1} - p_n).$$

A lot has been conjectured about large prime gaps; much less has been rigorously proved. Today's best known results on the growth of $G(x)$ as $x \to \infty$ are as follows:

$$A\,\frac{\log x \log\log x \log\log\log\log x}{\log\log\log x} \;<\; G(x) \;<\; Bx^{0.525},$$

with some positive constants A and B. The upper bound is due to Baker, Harman & Pintz [1], and the lower bound to Ford, Green, Konyagin, Maynard & Tao [6]. (Computations suggest that the above double inequality holds with $A = B = 1$ for all $x \ge 153$, while the lower bound holds with $A = 1$ wherever the left-hand side expression is defined.)

The notion of prime gap admits a natural generalization. Given an increasing integer sequence (S), we can consider gaps $p' - p$ between primes p and p' both of which are in (S), under the condition that $p < p'$ and there are no other primes in (S) between p and p'. Maximal gaps and first occurrence gaps between primes in (S) are also defined in a natural way, similar to the above.

In our recent work [13] we investigated the statistical properties of maximal gaps in certain increasing subsequences of the prime numbers. In this paper we turn our attention to a related, more numerous family of prime gaps: the *first occurrences* of gaps of a particular size. As a sequence (S) of interest, here we will choose an arithmetic progression (P): $r + nq$, $n = 0, 1, 2, 3, \dots$, with $\gcd(q, r) = 1$. It is plain that the first-occurrence gaps include, as a subsequence, all maximal gaps between primes $p \equiv r \pmod q$. We will see that maximal gaps and first-occurrence gaps between primes in (P) share certain statistical properties.

If we limit ourselves to studying the maximal and first-occurrence gaps in the sequence of *all primes*, we will find that the available data are quite scarce. As of 2019, we know only 745 first-occurrence gaps between primes below $2^{64} \approx 1.84 \cdot 10^{19}$; of these first occurrences, only 80 gaps are maximal [17]. That's one of the compelling reasons to study large gaps between primes in *residue classes*, i.e., in arithmetic progressions (P): $r + nq$. If the value of q used as the common difference of progression (P) is "not too small", we get *plenty of data* to study large prime gaps. That is, we get many sequences of first-occurrence gaps corresponding to progressions $r + nq$, for *the same fixed* q, which enables us to focus on common features of these sequences. One such feature is the common histogram of (appropriately rescaled) sizes of first-occurrence gaps. Other interesting features are the *average* numbers of maximal gaps and first-occurrence gaps between primes in (P) not exceeding x.

1.1 Notation

p_n	the n-th prime; $\{p_n\} = \{2, 3, 5, 7, 11, \ldots\}$
$q,\ r$	coprime integers, $1 \le r < q$
$(\mathrm{P}) = (\mathrm{P})_{q,r}$	the arithmetic progression $\ r,\ r+q,\ r+2q,\ r+3q, \ldots$
$P_f(d; q, r)$	the prime starting the first occurrence of gap d between primes in (P)
$P'_f(d; q, r)$	the prime ending the first occurrence of gap d between primes in (P)
$p_f(d)$	the prime starting the first occurrence of gap d in the sequence of all primes
$\gcd(m, n)$	the greatest common divisor of m and n
$\mathrm{LCM}(m, n)$	the least common multiple of m and n
$\lfloor x \rfloor$	the floor function: the greatest integer $\le x$
$\lceil x \rceil$	the ceiling function: the least integer $\ge x$
$\varphi(q)$	Euler's totient function (OEIS A000010)
$\mathrm{Gumbel}(x; \alpha, \mu)$	the Gumbel distribution cdf: $\ \mathrm{Gumbel}(x; \alpha, \mu) = e^{-e^{-\frac{x-\mu}{\alpha}}}$
$\mathrm{Exp}(x; \alpha)$	the exponential distribution cdf: $\ \mathrm{Exp}(x; \alpha) = 1 - e^{-x/\alpha}$
α	the *scale parameter* of exponential/Gumbel distributions, as applicable
μ	the *location parameter* (*mode*) of the Gumbel distribution
γ	the Euler–Mascheroni constant: $\ \gamma = 0.57721\ldots$
Π_2	the twin prime constant: $\ \Pi_2 = 0.66016\ldots$
$\log x$	the natural logarithm of x
$\operatorname{li} x$	the logarithmic integral of x: $\ \operatorname{li} x \,=\, \int_0^x \frac{\mathrm{d}t}{\log t} \,=\, \int_2^x \frac{\mathrm{d}t}{\log t} + 1.04516\ldots$
	Prime counting functions:
$\pi(x)$	the total number of primes $p_n \le x$
$\pi(x; q, r)$	the total number of primes $p = r + nq \le x$
	Gap measure functions:
$G(x)$	the maximal gap between primes $\le x$: $\ G(x) = \max_{p_{n+1} \le x}(p_{n+1} - p_n)$
$G_{q,r}(x)$	the maximal gap between primes $p = r + nq \le x$
$d_{q,r}(x)$	the latest first-occurrence gap between primes $p = r + nq \le x$ (sect. 3)
$R(n, q, r)$	size of the n-th record (maximal) gap between primes in (P)
$S(n, q, r)$	size of the n-th first-occurrence gap between primes in (P)
CSG	the Cramér–Shanks–Granville ratio for gap $p' - p$: $\ \mathrm{CSG} = \dfrac{p' - p}{\varphi(q) \log^2 p'}$
$a(q, x)$	the expected average gap between primes in (P): $\ a(q, x) = x\varphi(q) / \operatorname{li} x$
$T_0,\ T_f,\ T_m$	trend functions predicting the growth of large gaps (sect. 2)
	Gap counting functions:
$N_{q,r}(x)$	the number of maximal gaps $G_{q,r}$ in (P) with endpoints $p \le x$
$N'_{q,r}(x)$	the number of first-occurrence gaps in (P) with endpoints $p \le x$
$\tau_{q,r}(d, x)$	the number of gaps of a given even size $d = p' - p$ between successive primes $p, p' \equiv r \pmod{q}$, with $p' \le x$; $\ \ \tau_{q,r}(d, x) = 0\ $ if $q \nmid d$ or $2 \nmid d$.

1.2 Preliminaries

The following theorems and conjectures provide a broader context for our work on large prime gaps.

The prime number theorem states that the number of primes not exceeding x is asymptotic to the logarithmic integral $\operatorname{li} x$:

$$\pi(x) \;\sim\; \operatorname{li} x \qquad \text{as } x \to \infty. \tag{1}$$

The Riemann hypothesis implies that the error term in (1) is small:

$$\pi(x) - \operatorname{li} x \;=\; O\big(x^{1/2+\varepsilon}\big) \qquad \text{for any } \varepsilon > 0;$$

that is, the numbers $\pi(x)$ and $\lfloor \operatorname{li} x \rfloor$ almost agree in the left half of their digits.

Let $q > r \ge 1$ be fixed coprime integers, and consider the arithmetic progression

$$\text{(P)} \quad r,\; r+q,\; r+2q,\; r+3q,\; \ldots$$

Dirichlet's theorem on arithmetic progressions [5] establishes that there are infinitely many primes in progression (P) whenever $\gcd(q,r) = 1$.

The prime number theorem for arithmetic progressions [9] states that the number of primes in progression (P) not exceeding x is asymptotically equal to $1/\varphi(q)$ of the total number of primes $\le x$, that is,

$$\pi(x;q,r) \;\sim\; \frac{\pi(x)}{\varphi(q)} \;\sim\; \frac{\operatorname{li} x}{\varphi(q)} \qquad \text{as } x \to \infty, \tag{2}$$

where $\varphi(q)$ is Euler's totient function. Under the *Generalized Riemann Hypothesis* [9, p. 253]

$$\pi(x;q,r) - \frac{\operatorname{li} x}{\varphi(q)} \;=\; O\big(x^{1/2+\varepsilon}\big) \qquad \text{for any } \varepsilon > 0.$$

Polignac's conjecture [20] states that every gap of an even size $d = 2n$, $n \in \mathbb{N}$, actually occurs between consecutive primes infinitey often. (In section 4 we generalize Polignac's conjecture to gaps of size $n \cdot \mathrm{LCM}(2,q)$ between primes in progression (P); see Conjecture 6.)

Regarding the behavior of the function $G(x)$ — the maximal prime gap up to x — Cramér conjectured in the 1930s that $G(x) = O(\log^2 x)$ [4]; Shanks set forth a stronger hypothesis: $G(x) \sim \log^2 x$ [26].

Denote by $G_{q,r}(x)$ the maximal gap between primes $\le x$ in progression (P).

The generalized Cramér conjecture states that almost all maximal gaps $G_{q,r}(x)$ satisfy

$$G_{q,r}(x) \;<\; \varphi(q) \log^2 x. \qquad \text{[13, eq.(34)]} \tag{3}$$

The generalized Shanks conjecture is similar: almost all maximal gaps $G_{q,r}(x)$ satisfy

$$G_{q,r}(x) \;\sim\; \varphi(q) \log^2 x. \qquad \text{[13, eq.(35)]} \tag{4}$$

2 The growth trend of large gaps

In this section we introduce three trend functions useful in describing the growth and distribution of large gaps between primes in arithmetic progression (P): $r + nq$. These trend functions are asymptotically equivalent to $\varphi(q)\log^2 x$ and differ only in lower-order terms.

- The function $T_0(q,x)$ is called a *baseline trend*. Roughly speaking, for large enough x, this trend curve separates typical sizes of maximal gaps from typical sizes of non-maximal first-occurrence gaps; see sect. 2.1.
- The function $T_m(q,x)$ will give us an estimate of the most probable maximal gap sizes. We have $T_m(q,x) \ge T_0(q,x)$; see sect. 2.2.
- The function $T_f(q,x)$ will give us an estimate of the most probable first-occurrence gap sizes. For large x, we have $T_f(q,x) < T_0(q,x)$; see sect. 2.3.

Motivated by the prime number theorem for arithmetic progressions (2), we give the following estimate $a(q,x)$ of the average gap between primes in (P), to be used in trend functions.

Definition 1. The *expected average gap* between primes $p \le x$ in progression (P) is

$$a(q,x) \;=\; \frac{x\varphi(q)}{\operatorname{li} x}, \tag{5}$$

where $\varphi(q)$ is Euler's totient function, and $\operatorname{li} x$ is the logarithmic integral.

2.1 The baseline trend $T_0(q,x)$

We now define a trend function that will play a central role in this work.

Definition 2. The *baseline trend* $T_0(q,x)$ for large gaps between primes in (P) is

$$T_0(q,x) \;=\; a(q,x)\,\log\frac{\operatorname{li} x}{a(q,x)}, \tag{6}$$

where $a(q,x)$ is given by (5), and x is large enough, so that $\frac{\operatorname{li} x}{a(q,x)} > 1$.

The expression in the right-hand side of (6) is a concise form of [13, eq. (33)] in which we choose a constant term[1] $b = \log\varphi(q)$. Thus, by definition we have

$$T_0(q,x) \;=\; \frac{x\varphi(q)}{\operatorname{li} x}\left(2\log\frac{\operatorname{li} x}{\varphi(q)} - \log\frac{x}{\varphi(q)}\right). \tag{7}$$

(Equations (6) and (7) can also be viewed as a generalization of the trend equation derived in [31, 30] for maximal prime gaps $G(x)$, that is, for the particular case $q = 2$.)

[1]The choice of $b = \log\varphi(q)$ for use in [13, eq. (33)] reflects our heuristic expectation that, for large x, maximal gaps between primes $\le x$ in (P) should depend primarily on x and $a(q,x)$. Moreover, this choice is supported by extensive numerical results; cf. [13, sect. 3.1].

Remark 3. The baseline trend T_0 defined in (6) has the following properties:
(i) $T_0(q,x)$ is a continuous and smooth function of x for every fixed q.
(ii) $T_0(q,x)$ does not depend on the choice of r in progression (P).
(iii) $T_0(q,x)$ does not use unknown parameters determined a posteriori.
(iv) By way of comparison, for exponentially distributed *random* gaps between rare events, with mean gap α and cdf $\mathrm{Exp}(\xi;\alpha) = 1 - e^{-\xi/\alpha}$, the trend formula for maximal gaps is $g \approx \alpha \log \frac{x}{\alpha}$ (cf. [11, sect. 3.3]). Note the absence of $\operatorname{li} x$, in contrast to (6).

Clearly, as $x \to \infty$ we have

$$a(q,x) \;\lesssim\; \varphi(q) \log x, \tag{8}$$

$$T_0(q,x) \;\lesssim\; \varphi(q) \log^2 x. \tag{9}$$

Numerical results. We experimented with arithmetic progressions (P): $r + nq$ for many different coprime pairs (q,r). Invariably, we found that the majority of maximal gaps between primes $\le x$ in (P) have sizes *above* the baseline trend curve $T_0(q,x)$; that is, we usually have $G_{q,r}(x) > T_0(q,x)$. At the same time, for large enough x, a significant proportion of non-maximal first-occurrence gap sizes are *below* the curve $T_0(q,x)$.

2.2 The trend $T_m(q,x)$ of maximal gaps

Most probable *maximal* gaps $G_{q,r}(x)$ are close to the following trend [13, eqs. (33), (45)]:

$$T_m(q,x) \;=\; T_0(q,x) + \mathscr{E}_m(q,x), \tag{10}$$

where the error term $\mathscr{E}_m(q,x)$ is nonnegative and given by this empirical formula:

$$\mathscr{E}_m(q,x) \;\approx\; \frac{b_1 \log \varphi(q)}{(\log\log x)^{b_2}} \cdot a(q,x). \tag{11}$$

For $q = 2$, formula (11) gives $\mathscr{E}_m(2,x) = 0$. Indeed, we found that the baseline trend $T_0(2,x)$, even *without* an error term, satisfactorily describes the most probable sizes of maximal prime gaps $G(x)$. (Another reasonably good choice of the error term in (10) for $q = 2$ is $\mathscr{E}_m(2,x) = ca(q,x)$ with a constant $c \in [0, \frac{1}{2}]$.)

For $q > 2$, we found that the error term $\mathscr{E}_m(q,x)$ is positive, and it is best to determine the parameters b_1 and b_2 in (11) *a posteriori*. However, for $x \in [10^7, 10^{14}]$ and $q \in [10^2, 10^5]$, choosing

$$b_1 = 4, \qquad b_2 = 2.7 \tag{12}$$

yields a "good enough" trend curve for typical maximal gap sizes. This choice of b_1, b_2 works better when q is prime or semiprime. See [13] for further details on maximal gaps.

2.3 The trend $T_f(q,x)$ of first-occurrence gaps

For the trend equation to better describe the most probable *first-occurrence* gap sizes, we add a lower-order correction term to $T_0(q,x)$:

$$T_f(q,x) \;=\; T_0(q,x) + \mathscr{E}_f(q,x). \tag{13}$$

Based on extensive numerical data, we find that the term $\mathscr{E}_f(q,x)$ is eventually negative and given by this empirical formula:

$$\mathscr{E}_f(q,x) \;\approx\; a(q,x)\cdot(c_0 - c_1 \log\log x), \tag{14}$$

where $a(q,x)$ is defined by (5).

Like with $T_m(q,x)$, it is best to determine the parameters c_0 and c_1 in (14) *a posteriori*. However, in some special cases, we were able to find empirical estimates for c_0 and c_1.

Special cases:

- If q is a *prime* ≥ 5, the following empirical formulas for parameters

$$\begin{aligned} c_0 &= c_0(q) \;\approx\; 2.18\,(\log \mathrm{LCM}(2,q))^{0.58}, \\ c_1 &= c_1(q) \;\approx\; 1.18\,(\log \mathrm{LCM}(2,q))^{0.364} \end{aligned} \tag{15}$$

  work well in the term $\mathscr{E}_f(q,x)$ (14), for $x \in [10^7, 10^{14}]$ and $q \in [5, 10^5]$.

- If q is an *even semiprime* ≥ 10, it is plain that we deal with the same sequences of even first-occurrence gaps as above, so we can use the same formulas (15).

- For $q = 2$ (gaps in the sequence of all primes), the parameters

$$c_0 = 3, \qquad c_1 = 1.58 \tag{16}$$

  are close to optimal in the term $\mathscr{E}_f(2,x)$, at least for $x < 2^{64}$.

Numerical results. Using PARI/GP [19] we performed computational experiments with progressions $(\mathrm{P}) = (\mathrm{P})_{q,r}$ for many different values of $q \in [2, 10^5]$. Figure 1 shows the sizes of first-occurrence gaps between primes in twenty progressions (P), for $q = 211$ and $r \in [1, 20]$. Results for other values of q look similar to Fig. 1. All our numerical results show that trend curves of the form (13), (14) satisfactorily describe the growth of typical first-occurrence gaps between primes in progressions (P).

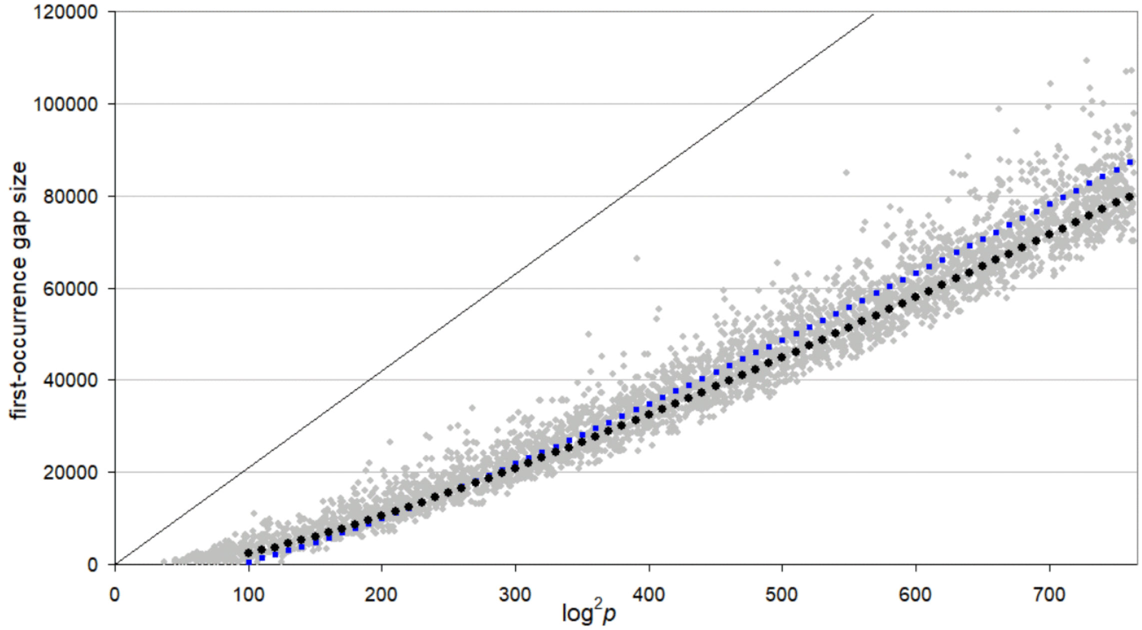

Figure 1: First-occurrence gaps $d_{q,r}$ between primes $p = r + nq \le 10^{12}$ for $q = 211$, $r \in [1, 20]$. Black curve: trend T_f (13)–(15); blue curve: baseline trend T_0 (6); top line: $y = \varphi(q)\log^2 p$. The vast majority of *maximal* gaps stay above T_0, while a growing proportion of non-maximal first-occurrence gaps are observed below T_0.

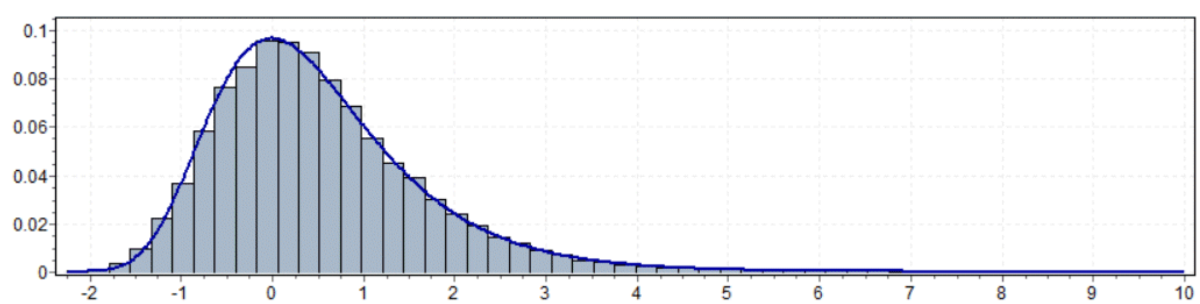

Figure 2: Histogram of rescaled values u (17) for the first-occurrence gaps between primes $p = r + nq \in [10^7, 10^{12}]$ for $q = 211$ and all $r \in [1, 210]$. Bins: 53, bin size ≈ 0.23. Blue curve: the best-fit Gumbel distribution (pdf) with scale $\alpha = 0.87692$ and mode $\mu = -0.00902$.

3 The distribution of first-occurrence gap sizes

Extensive numerical data allows us to observe that typically a first-occurrence gap is also the largest gap between primes in the interval $[x, x + x/(\log x)^{1+\varepsilon}]$, for some $\varepsilon > 0$. This invites the question (cf. [10], [13]): do first-occurrence gap sizes, after an appropriate rescaling transformation, obey the same distribution as maximal gap sizes — the Gumbel extreme value distribution?

Let $d = d_{q,r}(x)$ denote the size of the first-occurrence gap between primes $p \in [1, x] \cap (\text{P})$; specifically, the gap $d_{q,r}(x)$ refers to the first occurrence *closest to* x on the interval $[1, x]$. Infinitely many distinct values of $d_{q,r}(x)$ are maximal gaps, for which $d_{q,r}(x) = G_{q,r}(x)$. At the same time, infinitely many distinct values of $d_{q,r}(x)$ are *not* maximal gaps, and for these first occurrences we have $d_{q,r}(x) < G_{q,r}(x)$.

Rescaling transformation. Extreme value theory (EVT) motivates the following rescaling transformation (cf. [13, sect. 3.2]):

$$\text{gap size } d_{q,r}(x) \quad \mapsto \quad u = \frac{d_{q,r}(x) - T_f(q, x)}{a(q, x)}, \tag{17}$$

where $a(q, x)$ is the expected average gap (5), $T_f(q, x)$ is the trend function of first-occurrence gaps (13), and x runs through all end-of-gap primes in a given table of first-occurrence gaps. Every distinct gap size $d_{q,r}(x)$ is counted only once and mapped to its rescaled value u.

Figure 2 shows a combined histogram of rescaled values u for first-occurrence gaps between primes in progressions (P) for $q = 211$ and all $r \in [1, 210]$. We can see at once that the histogram is skewed to the right. A good fit is the Gumbel extreme value distribution — which typically occurs in statistics as the distribution of maxima of i.i.d. random variables with an initial *unbounded light-tailed* distribution.

For best-fit Gumbel distributions, we found that the Kolmogorov–Smirnov (KS) goodness-of-fit statistic was usually not much better (and sometimes worse) than the corresponding KS statistic measured for the data subset including *maximal gaps only*. In both cases (all first occurrences vs. maximal gaps only) the scale parameter α of best-fit Gumbel distributions was in the range $\alpha \in [0.7, 1]$. In both cases, when we moved from smaller to larger end-of-gap primes, the scale α of best-fit Gumbel distribution appeared to slowly grow towards 1.

Among three-parameter distributions, a very good fit for first-occurrence gap histograms is the *Generalized Extreme Value* (GEV) distribution. Typical best-fit GEV distributions for rescaled values (17) have a small negative *shape parameter*, usually in the interval $[-0.04, 0]$. Recall that the Gumbel distribution is a GEV distribution whose shape parameter is exactly zero. From extreme value theory we also know that the GEV distribution of maxima with a negative shape parameter occurs for i.i.d. random variables with an initial distribution *bounded from above*. On the other hand, if we fitted a GEV distribution to a data subset including *maximal gaps only*, then the resulting shape parameter was very close to zero, which is typical for random variables with an *unbounded light-tailed* distribution (the Gumbel type).

Our observations are compatible with the existence of a Gumbel limit law for (appropriately rescaled) maximal gaps, as well as for first-occurrence gaps between primes in progressions (P). However, the convergence to the hypothetical Gumbel limit law appears to be better for data sets comprising maximal gaps only, as opposed to data sets including all first-occurrence gaps (in a given range of primes in progressions (P) for a given q).

An alternative hypothesis is that the Gumbel limiting distribution exists for rescaled maximal gaps, but not for first-occurrence gaps. Of course it is also possible that there is no limiting distribution at all, and the Gumbel distribution is simply a good approximation of the rescaled gap values.

4 When do we expect the first occurrence of gap d?

Let d be the size of a gap between primes in progression (P): $r + nq$, and denote by

$$P_f(d; q, r) \quad \text{and} \quad P'_f(d; q, r)$$

the primes that, respectively, start and end the *first occurrence* of gap d. So we have

$$d \;=\; P'_f(d; q, r) - P_f(d; q, r).$$

Conjecture 4. Every even gap that is allowed to occur (by divisibility considerations) *does actually occur.* More formally: for every pair of coprime integers (q, r), $q > r \geq 1$, and every $d = k \cdot \mathrm{LCM}(2, q)$, $k \in \mathbb{N}$, we have

$$P_f(d; q, r) < \infty.$$

Conjecture 5. Let d be a gap between primes in (P). There exists a constant C such that infinitely often we have

$$e^{\sqrt{d/\varphi(q)}} \;<\; P_f(d; q, r) \;<\; C\sqrt{d}\,e^{\sqrt{d/\varphi(q)}}, \tag{18}$$

and the difference $P_f(d; q, r) - C\sqrt{d}\,e^{\sqrt{d/\varphi(q)}}$ changes its sign infinitely often as $d \to \infty$.

Conjecture 6. *Generalization of Polignac's conjecture for an arithmetic progression* (P): Every gap of size $n \cdot \mathrm{LCM}(2, q)$, $n \in \mathbb{N}$, occurs *infinitely often* between successive primes in progression (P).

For maximal gaps between primes in (P), we also state the following *stronger* conjectures.

Conjecture 7. Let $d = G_{q,r}(p')$ be a *maximal gap* between primes in (P). Then there exists a constant C such that a *positive proportion* of maximal gaps satisfy the double inequality (18), and the difference $P_f(d; q, r) - C\sqrt{d}\,e^{\sqrt{d/\varphi(q)}}$ changes its sign infinitely often as $d \to \infty$.

Conjecture 8. Let $d = G_{q,r}(p')$ be a *maximal gap* between primes in (P). Then, as $d \to \infty$, a *positive proportion* of maximal gaps satisfy

$$P_f(d;q,r) \asymp \sqrt{d}\, e^{\sqrt{d/\varphi(q)}}. \tag{19}$$

In other words, there are constants $C_0, C_1 > 0$ such that a positive proportion of maximal gaps satisfy the double inequality

$$C_0\sqrt{d}\, e^{\sqrt{d/\varphi(q)}} < P_f(d;q,r) < C_1\sqrt{d}\, e^{\sqrt{d/\varphi(q)}}. \tag{20}$$

Computations suggest that if we take $C_0 = \frac{1}{10}$, $C_1 = 10$, then the vast majority of maximal gap sizes will satisfy (20); a sizeable proportion of non-maximal first-occurrence gaps will also be found within the bounds (20).

How did we arrive at the estimates (18)–(20)? The left-hand side $e^{\sqrt{d/\varphi(q)}}$ in (18) stems from the conjecture [13, eq. (34)] that *almost all* maximal gaps between primes in (P) satisfy

$$G_{q,r}(p) < \varphi(q)\log^2 p.$$

(This is our generalization of Cramér's conjecture [4].)

To see why we have $C\sqrt{d}\, e^{\sqrt{d/\varphi(q)}}$ in the right-hand side of (18)–(20), consider the function

$$\tilde{P}(d,q) = \sqrt{d}\, e^{\sqrt{d/\varphi(q)}}. \tag{21}$$

For any fixed $q \ge 2$, one can check that

$$\lim_{x\to\infty} \frac{\tilde{P}(T_0(q,x),q)}{x} = e^{-1/2} \approx 0.60653. \tag{22}$$

That is, for large d and x, the function $e^{1/2}\tilde{P}(d,q)$ is "almost inverse" of $T_0(q,x)$ in (6).

Remark 9. We do not know whether the lower bound in (18) is reversed infinitely often or finitely often. For the special case $q = 2$ (gaps in the sequence of all primes), a heuristic argument of Granville [8] leads to $\limsup\limits_{x\to\infty} \frac{G(x)}{\log^2 x} \ge 2e^{-\gamma} \approx 1.1229$. This suggests that, for first-occurrence prime gaps, the lower bound in (18) is reversed infinitely often. However, it is quite difficult to find examples of progressions (P): $r + nq$ with exceptionally early first occurrences of gaps d such that $P'_f(d;q,r) < e^{\sqrt{d/\varphi(q)}}$ and the Cramér–Shanks–Granville ratio CSG $= \frac{d_{q,r}(x)}{\varphi(q)\log^2 x} > 1$. We know just a few examples of maximal gaps of this kind [13, Table 1], [21, 22]; and all these exceptional maximal gaps are smaller than q^2. We have never seen examples of sign reversal of the lower bound in (18) (CSG > 1) for *non-maximal* first-occurrence gaps in (P). Note also that Sun [27, conj. 2.3] proposed a hypothesis similar to Firoozbakht's conjecture for gaps between primes in (P), which would imply (at most) a finite number of such sign reversals for any given progression (P) with an even q.

5 A detour: generalization of Brun's constants

We will now give another (less direct) heuristic way of deriving the estimate $C\sqrt{d}\,e^{\sqrt{d/\varphi(q)}}$ in the right-hand side of (18). Our approach is to estimate the sum of reciprocals of prime pairs $(p,\,p+d)$ separated by a given fixed gap d. (Wolf [29] used this heuristic approach to treat the case $q=2$, obtaining the estimate[2] $\sqrt{d}\,e^{\sqrt{d}}$ for the first occurrence of gap d.)

First, let us recall some important definitions. *Twin primes* are pairs of prime numbers $(p,\,p+2)$ separated by the smallest possibe gap 2. *Cousin primes* are pairs of prime numbers $(p,\,p+4)$ separated by gap 4.

Brun [3] proved in 1919 that the series consisting of reciprocal twin primes converges. Brun's constant B_2 for twin primes is the sum of reciprocals:

$$B_2 \;=\; \left(\frac{1}{3}+\frac{1}{5}\right)+\left(\frac{1}{5}+\frac{1}{7}\right)+\left(\frac{1}{11}+\frac{1}{13}\right)+\ldots \;\approx\; 1.90216 \quad [7,\,15,\,16,\,24].$$

A generalization of Brun's theorem exists for series of reciprocal values of prime pairs $(p,\,p{+}d)$ separated by *any fixed gap* d [25]. For example, Brun's constant B_4 for cousin primes (with the pair $(3,7)$ omitted) is

$$B_4 \;=\; \left(\frac{1}{7}+\frac{1}{11}\right)+\left(\frac{1}{13}+\frac{1}{17}\right)+\left(\frac{1}{19}+\frac{1}{23}\right)+\ldots \;\approx\; 1.19704 \qquad [28].$$

Note that twin primes $p,\,p+2$ are always consecutive. Except for the pair $(3,7)$, primes $p,\,p+4$ are also necessarily consecutive. If $d\ge 6$, however, there may also be other primes between the primes p and $p+d$. In what follows, we will consider gaps $d\ge 6$.

Suppose that primes p and p' are in the residue class $r \pmod q$, $p<p'$, and there are *no other primes* in this residue class between p and p'. If $d=n\cdot\mathrm{LCM}(2,q)$, then the number of gaps of size $d=p'-p$ between primes $p,p'\equiv r \pmod q$, with $p'\le x$, is roughly

$$\tau_{q,r}(d,x) \;\approx\; C_2\prod_{\substack{p|d\\p>2}}\frac{p-1}{p-2}\cdot\frac{\pi^2(x)}{\varphi^2(q)x}\,e^{-\frac{d\cdot\pi(x)}{\varphi(q)x}} \qquad [13,\text{ eq. }(30)], \tag{23}$$

where p runs through odd prime factors of d,

$$C_2=\frac{c}{s},\qquad c=\mathrm{LCM}(2,q),\qquad s=\operatorname*{mean}_{d=nc}\prod_{\substack{p|d\\p>2}}\frac{p-1}{p-2}=\Pi_2^{-1}\prod_{\substack{p|q\\p>2}}\frac{p}{p-1}, \tag{24}$$

and $\Pi_2=\prod\limits_{p>2}\frac{p(p-2)}{(p-1)^2}\approx 0.66016$ is the twin prime constant. In particular, $s=\Pi_2^{-1}\approx 1.51478$ if q is a power of 2; see *Appendix*. Note that

$$\tau_{q,r}(d,x) \;=\; 0 \quad \text{ if } 2\nmid d \;\text{ or }\; q\nmid d. \tag{25}$$

[2]The preprint [29] employs the "physical" notation where the relation $f\sim g$ is a shorthand for "the functions f and g have the same order of magnitude." Thus $\sqrt{d}\,e^{\sqrt{d}}$ is just an order-of-magnitude estimate.

Denote by $\mathscr{T}_d(q,r)$ the set of primes p, p' at both ends of the gaps d counted in (23):

$$\mathscr{T}_d(q,r) \;=\; \{p,p' :\; p'-p=d \;\text{ and }\; p,p' \equiv r \bmod q\}. \tag{26}$$

Consider the sum of reciprocals of all primes in $\mathscr{T}_d(q,r)$:

$$B_d(q,r) \;=\; \sum_{p\,\in\mathscr{T}_d(q,r)} \frac{1}{p}. \tag{27}$$

We adopt the rule that if a given gap d appears twice in a row: $d = p'-p = p''-p'$, then the corresponding middle prime p' is counted twice. The real numbers $B_d(q,r)$ defined by (27) can be called *the generalized Brun constants* for residue class r (mod q).

Let us define the partial (finite) sums:

$$B_d(x;q,r) \;=\; \sum_{\substack{p\in\mathscr{T}_d(q,r)\\ p\le x}} \frac{1}{p}. \tag{28}$$

Hereafter we will work with rough estimates of partial sums (28). To distinguish the actual partial sum $B_d(x;q,r)$ from its estimated value, we will write $\mathscr{B}_d(x;q)$ for the estimate. Likewise, for a rough estimate of the constant (27), we will write $\mathscr{B}_d(\infty;q)$. Our estimates $\mathscr{B}_d(\,\cdot\,;q)$ will be independent of r.

Given a gap size $d=p'-p$, observe that the density of pairs $(p,p') \subset \mathscr{T}_d(q,r)$ near x is roughly $\tau_{q,r}(d,x)/x$. Putting $\pi(x) \approx x/\log(x)$ in equation (23), we obtain

$$\mathscr{B}_d(x;q) \;\approx\; \sum_{p\in\mathscr{T}_d(q,r)} \frac{1}{p} \;-\; \sum_{\substack{p\in\mathscr{T}_d(q,r)\\ p>x}} \frac{1}{p} \;\approx\; \mathscr{B}_d(\infty,q) - 2C_2 \prod_{p|d} \frac{p-1}{p-2} \int_x^\infty \frac{e^{-\frac{d}{\varphi(q)\log u}}}{\varphi^2(q)\,u\log^2 u}\,\mathrm{d}u. \tag{29}$$

After the substitution $v=\frac{d}{\varphi(q)\log u}$ the integral (29) can be calculated explicitly:

$$\mathscr{B}_d(x;q) \;\approx\; \mathscr{B}_d(\infty;q) + \frac{2C_2}{\varphi(q)d} \prod_{p|d} \frac{p-1}{p-2} \left(e^{-\frac{d}{\varphi(q)\log x}} - 1\right). \tag{30}$$

We will require that $\mathscr{B}_d(x;q) \to 0$ as $x \to 1^+$ (indeed, the actual partial sum $B_d(x;q,r)$ will be zero up to the first occurrence of the gap d). Taking the limit $x \to 1^+$ in (30) we obtain

$$\mathscr{B}_d(\infty;q) \approx \frac{2C_2}{\varphi(q)d} \prod_{p|d} \frac{p-1}{p-2}. \tag{31}$$

Then the estimate $\mathscr{B}_d(x;q)$, as a function of x for fixed q and d, has the form

$$\mathscr{B}_d(x;q) \approx \frac{2C_2}{\varphi(q)d} \prod_{p|d} \frac{p-1}{p-2}\, e^{-\frac{d}{\varphi(q)\log x}}. \tag{32}$$

Recall that, for $d = n \cdot \mathrm{LCM}(2,q)$, the mean value of $\prod_{p|d} \frac{p-1}{p-2}$ is s; see (23), (24). Therefore, we can skip the ratio $\prod_{p|d} \frac{p-1}{p-2}/s \approx 1$ and get

$$\mathscr{B}_d(x;q) \;\approx\; \frac{2c}{\varphi(q)d}\, e^{-\frac{d}{\varphi(q)\log x}} \;=\; \frac{A}{d}\, e^{-\frac{d}{\varphi(q)\log x}}, \tag{33}$$

where $c = \mathrm{LCM}(2,q)$ and $A = 2c/\varphi(q) = O(\log\log q)$; moreover[3] $A = O(1)$ for prime q.

Suppose that gap d occurs for the first time at $\xi = P_f(d;q,r)$. We can estimate ξ from the condition $\mathscr{B}_d(\xi;q) = 2/\xi$, so we have the following equation for ξ:

$$\frac{Ae^{-\frac{d}{\varphi(q)\log\xi}}}{d} \;=\; \frac{2}{\xi}. \tag{34}$$

Taking the log of both sides of (34) and discarding the small term $\log\frac{A}{2}$, we get a quadratic equation for $t = \log\xi$:

$$t^2 - t\log d \;=\; d/\varphi(q). \tag{35}$$

Its positive solution $t \approx \frac{1}{2}\log d + \sqrt{d/\varphi(q)}$ yields

$$\xi \;=\; P_f(d;q,r) \;\asymp\; \sqrt{d}\, e^{\sqrt{d/\varphi(q)}}. \tag{36}$$

Remark 10. Compare (36) to the formula for the first occurrence of gap d in the sequence of all primes, $p_f(d) \asymp \sqrt{d}\, e^{\sqrt{d}}$ [29]. It might seem that in an arithmetic progression (P) gaps of a given size appear much earlier (due to the division by $\varphi(q)$ under square root in the exponent). Note, however, that the "natural unit" of gaps in progressions (P) is larger than that for all primes; namely, gaps between primes in (P) have sizes $n \cdot \mathrm{LCM}(2,q)$, $n \in \mathbb{N}$.

6 How many first-occurrence gaps are there below x?

Using a modified version of our PARI/GP code from [13] we computed the mean numbers of first-occurrence gaps between primes $p = r + nq$ in intervals $[x, ex]$, $x = e^j$, $j = 1, 2, \ldots, 27$. Figure 3 shows the results of this computational experiment for $q = 17011$. For comparison, we also computed the corresponding mean numbers of record (maximal) gaps between primes $p = r + nq$ in the same set of intervals $[x, ex]$; the results are shown in Fig. 4.

We found that, for large enough x, the mean number of first-occurrence gaps between primes in $[x, ex]$ grows about as fast as a linear function of $\log x$; see Fig. 3. It is reasonable to expect that the *total* number $N'_{q,r}(x)$ of first-occurrence gaps between primes $\le x$ in progression (P) can be approximated by a quadratic function of $\log x$, and for large x we will have

$$N'_{q,r}(x) \;\approx\; \frac{T_0(q,x)}{\mathrm{LCM}(2,q)} \;\lesssim\; \frac{\varphi(q)\log^2 x}{\mathrm{LCM}(2,q)} \;=\; O(\log^2 x). \tag{37}$$

[3] We easily check that $A = 4$ when $q = 2$, and $A \le 6$ when q is an odd prime. On the other hand, one can also show that $A = O(\log\log q)$ when q is a primorial (which constitutes an extreme case; see [18]).

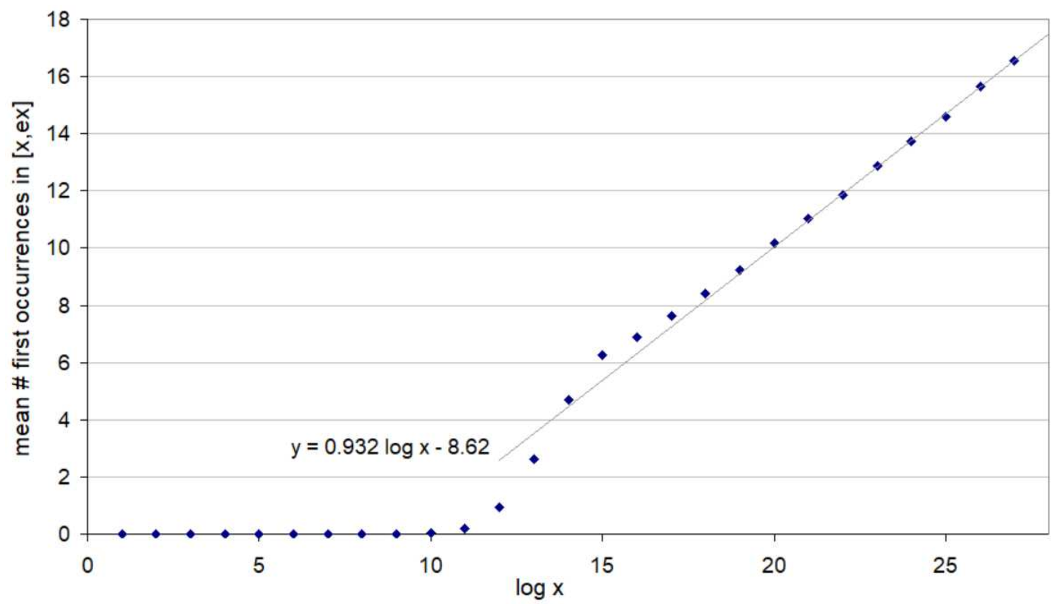

Figure 3: Mean number of first-occurrence gaps between primes $p = r + nq \in [x, ex]$, for $x = e^j$, $j = 1, 2, \ldots, 27$, with $q = 17011$. Averaging for all $r \in [1, 17010]$.

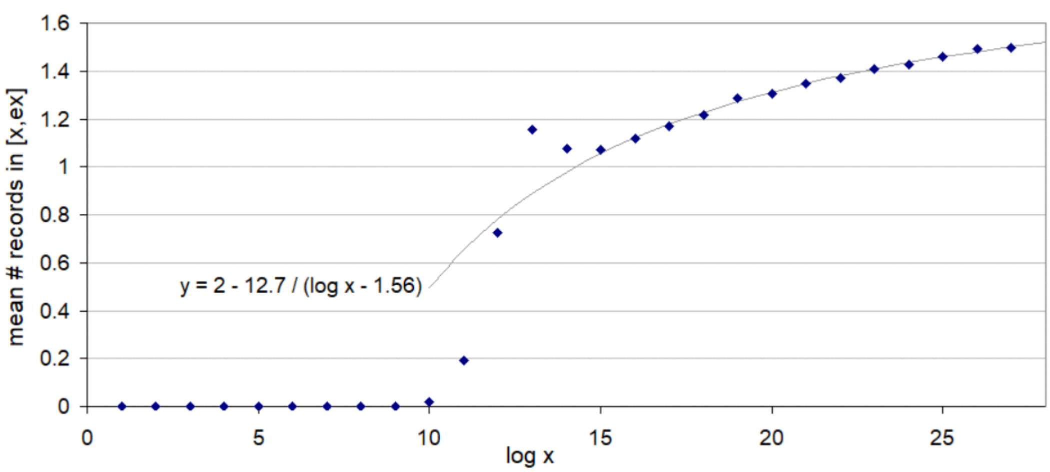

Figure 4: Mean number of record (maximal) gaps between primes $p = r + nq \in [x, ex]$, for $x = e^j$, $j = 1, 2, \ldots, 27$, with $q = 17011$. Averaging for all $r \in [1, 17010]$.

Thus the number of first-occurrence gaps between primes in (P) is asymptotically *much greater* than the number $N_{q,r}(x)$ of record (maximal) gaps in (P). Indeed, the latter seems to be only $O(\log x)$. More precisely, our computations suggest that the average number of maximal gaps observed in $[x, ex]$ is

$$\operatorname*{mean}_r \big(N_{q,r}(ex) - N_{q,r}(x)\big) \;\approx\; 2 - \frac{\kappa(q)}{\log x + \delta(q)}; \quad \text{see Fig. 4.} \tag{38}$$

Accordingly, we conjecture that the number of maximal gaps between primes $\le x$ in (P) is

$$N_{q,r}(x) \;\sim\; 2\log x \;=\; O(\log x) \qquad \text{as } x \to \infty. \tag{39}$$

(For a heuristic justification of the constant 2 in (38) and (39), see [12, 13].)

7 Maximal gaps and first occurrences as functions of their sequential number

As before, consider the arithmetic progression (P): $r,\ r+q,\ r+2q,\ r+3q,\ \ldots$.

Conjecture 11. Let $S(n; q, r)$ be the size of the n-th first-occurrence gap between primes in progression (P). Then the sizes $S(n; q, r)$ of almost all first-occurrence gaps satisfy

$$n \;\le\; S(n; q, r) \;\le\; 2nq\lceil \log^2 q\rceil. \tag{40}$$

Moreover, we expect that all "admissible" gap sizes occur early enough, so that

$$S(n; q, r) \;\approx\; n \cdot \mathrm{LCM}(2, q) \;=\; O_q(n) \qquad \text{as } n \to \infty. \tag{41}$$

For comparison, here is a similar conjecture for *maximal* gap sizes:

Conjecture 12. Let $R(n; q, r)$ be the size of the n-th record (maximal) gap between primes in (P). Then the sizes $R(n; q, r)$ of almost all maximal gaps satisfy [23]

$$\frac{\varphi(q)n^2}{6} \;<\; R(n; q, r) \;<\; \varphi(q)n^2 + (n+2)q\log^2 q. \tag{42}$$

The bound in the right-hand side of (42) was given earlier in [12]. As of 2019, we do not know any exceptions to (42). Heuristic reasoning [12, 13] suggests that

$$R(n; q, r) \;\approx\; \frac{\varphi(q)n^2}{4} \;=\; O_q(n^2) \qquad \text{as } n \to \infty. \tag{43}$$

Conjectures 11 and 12 are another way to restate our observation that first-occurrence gaps between primes in progression (P) are (eventually) much more numerous than maximal gaps.

Remark 13. If we substitute $n = 0$ in (42), we get that the "0th record gap" is less than $2q\log^2 q$, which can be interpreted as an almost-sure upper bound on the least prime in progression (P); cf. [14, sect.2]. That is, the "0th record gap" between primes in (P) is the distance from 0 to the least prime in (P), which is (almost always) bounded by $2q\log^2 q$.

8 Appendix

In this appendix we calculate the average value of the product

$$S(d) = \prod_{\substack{p|d \\ p>2}} \frac{p-1}{p-2} \tag{44}$$

when d runs through a given arithmetic progression, $d = r + nq$. So our goal is to find

$$\operatorname*{mean}_{d=r+nq} S(d) = \lim_{N\to\infty} \frac{1}{N} \sum_{n=1}^{N} S(r+nq).$$

For generality, in the appendix, q and r are not necessarily coprime. In particular, we will derive (24) for the case $d = nq$ $(r = 0)$. Bombieri and Davenport [2] proved that

$$\operatorname*{mean}_{d\in\mathbb{N}} S(d) = \operatorname*{mean}_{d\in\mathbb{N}} \prod_{\substack{p|d \\ p>2}} \frac{p-1}{p-2} = \Pi_2^{-1} = 1.51478\dots,$$

where Π_2 is the *twin prime constant* defined by

$$\Pi_2 = \prod_{p>2} \frac{p(p-2)}{(p-1)^2} = 0.66016\dots.$$

If, instead of averaging $S(d)$ over all natural numbers, we restrict the averaging process to an arithmetic progression $r+nq$, then the resulting average might become larger or smaller than Π_2^{-1} — or it might remain unchanged $(= \Pi_2^{-1})$. A few special cases are possible, depending on the values of q and r.

8.1 Basic cases: prime q

(i) If $q = 2$, we have $S(2n) = S(n)$ for all $n \in \mathbb{N}$. Therefore, for even d,

$$\operatorname*{mean}_{d=2n} S(d) = \operatorname*{mean}_{d\in\mathbb{N}} S(d) = \Pi_2^{-1}.$$

But this immediately implies that, for odd d, we must also have

$$\operatorname*{mean}_{d=2n+1} S(d) = \operatorname*{mean}_{d\in\mathbb{N}} S(d) = \Pi_2^{-1}.$$

(ii) Suppose $q = p'$ is an odd prime and $\gcd(p', r) = 1$. Let

$$\begin{aligned} \xi &= \xi(p') = \operatorname*{mean}_{d=np'} S(d) \\ \eta &= \eta(p') = \operatorname*{mean}_{d=r+np'} S(d). \end{aligned}$$

Observe that every term in progression $d = np'$ has the prime factor p'; so the factor $\frac{p'-1}{p'-2}$ is *always present* in the corresponding product (44). On the other hand, terms in progression $d = r + np'$ never have the prime factor p'; so the factor $\frac{p'-1}{p'-2}$ is *never present* in the corresponding product (44). All other odd prime factors p (resp., $\frac{p-1}{p-2}$), $p \neq p'$, are *sometimes* present in both progressions (resp., products), with probability $1/p$. Therefore, we require that

$$\xi = \eta \cdot \frac{p'-1}{p'-2}. \tag{45}$$

The factor $\frac{p'-1}{p'-2}$ in (45) is the same as in the definition of $S(d)$.

Note that there are $p'-1$ residue classes mod p' for which the mean values of $S(d)$ are η, and only one "special" residue class (0 mod p') for which the mean value of $S(d)$ is ξ. But the arithmetic average of all these p' mean values is equal to $\underset{d\in\mathbb{N}}{\operatorname{mean}} S(d)$, which is Π_2^{-1}:

$$\frac{1}{p'} \cdot \xi \ + \ \frac{p'-1}{p'} \cdot \eta \ = \ \Pi_2^{-1}. \tag{46}$$

Solving equations (45) and (46) together, we find

$$\xi \ = \ \underset{d=np'}{\operatorname{mean}} S(d) \ = \ \frac{p'}{p'-1} \cdot \Pi_2^{-1}, \tag{47}$$

$$\eta \ = \ \underset{d=r+np'}{\operatorname{mean}} S(d) \ = \ \frac{p'(p'-2)}{(p'-1)^2} \cdot \Pi_2^{-1}. \tag{48}$$

Example: for $q = 3$, we have

$$\underset{d=3n}{\operatorname{mean}} S(d) = \frac{3}{2}\Pi_2^{-1}, \qquad \underset{d=3n+1}{\operatorname{mean}} S(d) = \underset{d=3n+2}{\operatorname{mean}} S(d) = \frac{3}{4}\Pi_2^{-1}.$$

Formulas (47) and (48) encode the following

Factors Principle. For progressions $d = np'$ where each term is guaranteed to have a factor p', the average product $S(d)$ equals Π_2^{-1} multiplied by $\frac{p'}{p'-1} > 1$. For progressions $d = r + np'$ where each term *never* has the factor p', the average is Π_2^{-1} multiplied by $\frac{p'(p'-2)}{(p'-1)^2} < 1$.

8.2 Remaining cases: composite q

We now heuristically apply the above principle to composite values of q.

(A) q is a power of 2. (This case is similar to (i) in sect. 8.1.) In this case, for every odd prime p, terms of our arithmetic progression $r + nq$ span *all residue classes* modulo p. So here the average value of $S(d)$ remains unchanged:

$$\underset{d=r+2^k n}{\operatorname{mean}} S(d) \ = \ \Pi_2^{-1}.$$

Example: for $q = 4$, we have $\operatorname*{mean}_{d=4n} S(d) = \operatorname*{mean}_{d=4n+1} S(d) = \operatorname*{mean}_{d=4n+2} S(d) = \operatorname*{mean}_{d=4n+3} S(d) = \Pi_2^{-1}$.

(B) Suppose $q \neq 2^k$ is composite and $\gcd(q, r) = 1$. Here all terms of our arithmetic progression are not divisible by prime factors of q, while divisibility by all other primes is neither ensured nor precluded. We have

$$\operatorname*{mean}_{d=r+nq} S(d) \;=\; \Pi_2^{-1} \cdot \prod_{\substack{p|q \\ p>2}} \frac{p(p-2)}{(p-1)^2}.$$

Example: for $q = 15$ and $r = 1$, we have $\operatorname*{mean}_{d=15n+1} S(d) = \frac{3}{4} \cdot \frac{15}{16} \cdot \Pi_2^{-1} = \frac{45}{64}\Pi_2^{-1}$.

(C) Suppose $q \neq 2^k$ is composite and $r = 0$. All terms of our arithmetic progression are divisible by prime factors of q, while divisibility by all other primes is neither ensured nor precluded. We have

$$\operatorname*{mean}_{d=nq} S(d) \;=\; \Pi_2^{-1} \cdot \prod_{\substack{p|q \\ p>2}} \frac{p}{p-1}.$$

Example: for $q = 15$ and $r = 0$, we have $\operatorname*{mean}_{d=15n} S(d) = \frac{3}{2} \cdot \frac{5}{4} \cdot \Pi_2^{-1} = \frac{15}{8}\Pi_2^{-1}$.

(D) Suppose $q \neq 2^k$ is composite, $r \neq 0$, $\gcd(q, r) > 1$. (This case is, in a sense, a combination of the above cases.) Terms of our arithmetic progression $r + nq$ are divisible by common prime factors of q and r, but not by other prime factors of q; divisibility by all other primes is neither ensured nor precluded. We have

$$\operatorname*{mean}_{d=r+nq} S(d) \;=\; \Pi_2^{-1} \cdot \prod_{\substack{P|q,\, P|r \\ P>2}} \frac{P}{P-1} \cdot \prod_{\substack{p|q,\, p\nmid r \\ p>2}} \frac{p(p-2)}{(p-1)^2}. \tag{49}$$

Example: for $q = 30$ and $r = 3$, we have $\operatorname*{mean}_{d=30n+3} S(d) = \frac{3}{2} \cdot \frac{15}{16} \cdot \Pi_2^{-1} = \frac{45}{32}\Pi_2^{-1}$.

Remark. Formula (49) actually works for an arbitrary pair (q, r); it subsumes all preceding cases. Formulas like this can be derived not only in our setup related to the twin prime constant Π_2 but also for similar average products related to the Hardy–Littlewood k-tuple constants, as well as for other average products, e.g., $\operatorname*{mean}_{d=r+nq} \prod_{\substack{p|d \\ p>m}} \frac{p+a}{p+b}$.

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