A FAST ALGORITHM TO COMPUTE THE RAMANUJAN-DENINGER GAMMA-FUNCTION AND SOME NUMBER-THEORETIC APPLICATIONS

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Abstract. We introduce a fast algorithm to compute the Ramanujan-Deninger gamma function and its logarithmic derivative at positive values. Such an algorithm allows us to greatly extend the numerical investigations about the Euler-Kronecker constants $\mathfrak{G}_q$, $\mathfrak{G}_q^+$ and $M_q = \max_{\chi\neq\chi_0} |L'/L(1,\chi)|$, where q is an odd prime, χ runs over the primitive Dirichlet characters mod q, χ_0 is the trivial Dirichlet character mod q and $L(s,\chi)$ is the Dirichlet L-function associated to χ. Using such algorithms we obtained that $\mathfrak{G}_{50040955631} = -0.16595399\ldots$ and $\mathfrak{G}^+_{50040955631} = 13.89764738\ldots$ thus getting a new negative value for $\mathfrak{G}_q$.

Moreover we also computed $\mathfrak{G}_q$, $\mathfrak{G}_q^+$ and M_q for every odd prime q, $10^6 < q \leq 10^7$, thus extending the results in [17]. As a consequence we obtain that both $\mathfrak{G}_q$ and $\mathfrak{G}_q^+$ are positive for every odd prime q up to 10^7 and that $\frac{17}{20}\log\log q < M_q < \frac{5}{4}\log\log q$ for every odd prime $1531 < q \leq 10^7$. In fact the lower bound holds true for $q > 13$. The programs used and the results here described are collected at the following address `http://www.math.unipd.it/~languasc/Scomp-appl.html`.

1. Introduction

We introduce a fast algorithm to compute the Ramanujan-Deninger gamma function and its logarithmic derivative at positive real values. We then use such a new algorithm to efficiently compute $L'/L(1,\chi)$, where χ runs over the non trivial primitive Dirichlet characters mod q, q is an odd prime and $L(s,\chi)$ is the Dirichlet L-function associated to χ. Such a quantity is involved in several interesting number-theoretic problems like the evaluation of the Euler-Kronecker constants $\mathfrak{G}_q$ for the cyclotomic field $\mathbb{Q}(\zeta_q)$, ζ_q being a q-root of unity, the analogous problem for $\mathfrak{G}_q^+$ attached to $\mathbb{Q}(\zeta_q+\zeta_q^{-1})$, the maximal real subfield of $\mathbb{Q}(\zeta_q)$, and the study of the extremal values of $M_q = \max_{\chi\neq\chi_0} |L'/L(1,\chi)|$. We will give a detailed description of such problems in Section 4.

Following Deninger's notation in [3], we introduce now the functions we will work on. The main object is the *Ramanujan-Deninger* Gamma function $\Gamma_1(x) := \exp(R(x))$, $x > 0$, where

$$R(x) := -\frac{\partial^2}{\partial s^2}\zeta(s,x)|_{s=0}\,,$$

$\zeta(s,x)$ is the Hurwitz zeta function, $\zeta(s,x) = \sum_{n=0}^{+\infty}(n+x)^{-s}$ for $\Re(s) > 1$ and it is meromorphically extended to $s \in \mathbb{C}\setminus\{1\}$. We recall that $\zeta(s,1)$ is Riemann's zeta-function $\zeta(s)$. Using eq. (2.3.2) of [3], the R-function can be expressed for every $x > 0$ by

$$R(x) = -\zeta''(0) - S(x), \tag{1}$$

$$S(x) := 2\gamma_1 x + (\log x)^2 + \sum_{k=1}^{+\infty}\Big(\big(\log(k+x)\big)^2 - (\log k)^2 - 2x\frac{\log k}{k}\Big), \tag{2}$$

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where

$$\gamma_1 = \lim_{n\to+\infty}\Big(\sum_{k=1}^{n}\frac{\log k}{k} - \frac{(\log n)^2}{2}\Big), \quad \zeta''(0) = \frac{1}{2}\Big(-(\log 2\pi)^2 - \frac{\pi^2}{12} + \gamma_1 + \gamma^2\Big) \tag{3}$$

and γ is the Euler-Mascheroni constant. We introduced the S-function because in the applications we will see in Section 4 below the constant term $\zeta''(0)$ will play no role and hence we may focus our attention just on the S-function. We also have $S(1) = 0$ and $R(1) = -\zeta''(0)$.

A key point to be able to obtain the following results is that $R(x)$ is the unique solution in $(0, +\infty)$ of the difference equation $R(x+1) = R(x)+(\log x)^2$, with initial condition $R(1) = -\zeta''(0)$, which is convex in some interval $(A, +\infty)$, $A > 0$, see Theorem 2.3 of Deninger [3]. As a consequence the S-function too verifies a difference equation:

$$S(x + 1) = S(x) - (\log x)^2 \quad \text{for every } x > 0. \tag{4}$$

Another important ingredient to being able to derive our results is the following alternative definition of $S(x)$, $x > 0$, which is implicitly contained in eq. (2.12) of Deninger [3]. It is the analogue for S of *Plana's integral* for $\log\Gamma$, where $\Gamma(s)$, $s \in \mathbb{C} \setminus (-\mathbb{N})$, is Euler's Gamma function:

$$S(x) = 2\int_0^{+\infty}\Big((x-1)e^{-t} + \frac{e^{-xt} - e^{-t}}{1 - e^{-t}}\Big)\frac{\gamma + \log t}{t}\,\mathrm{d}t. \tag{5}$$

We introduce now the first derivative of $R(x)$, namely

$$\psi_1(x) := \frac{1}{2}R'(x) = \frac{1}{2}\frac{\Gamma_1'}{\Gamma_1}(x). \tag{6}$$

The factor $1/2$ in (6) is needed because Deninger, in its definition of $R(x)$, used an extra factor 2 and we need now to remove it to connect ψ_1 with the results proved by other authors. We also recall that generalised ψ-functions of this kind occur in Ramanujan's second notebook, see [1, Chapter 8, Entry 22]. Differentiating (2) we have

$$\psi_1(x) = -\gamma_1 - \frac{\log x}{x} - \sum_{k=1}^{+\infty}\Big(\frac{\log(k+x)}{k+x} - \frac{\log k}{k}\Big)$$

for $x > 0$. We also define

$$T(x) := \gamma_1 + \psi_1(x) \tag{7}$$

so that $T(1) = 0$. As before, we introduced the function $T(x)$ because the constant term γ_1 in the definition of ψ_1 will play no role in the applications contained in Section 4 below. Moreover, since $S'(x) = 2(\gamma_1 - T(x))$, it follows that

$$T(x) = \gamma_1 - \frac{1}{2}S'(x) \quad \text{and} \quad T(x+1) = T(x) + \frac{\log x}{x} \quad \text{for every } x > 0. \tag{8}$$

In our applications, see Section 4 below, we will need to evaluate S or T at some rational points contained in $(0, 1)$. A possible solution, used in [17], is to use the `intnum` and `sumnum` functions of PARI/GP [21] to numerically evaluate (2), (5) and (7). Here we show how to largely reduce the cost of this computation by introducing a new algorithm to obtain such quantities. Denoting as $\lceil y\rceil$ the least integer greater than or equal to $y \in \mathbb{R}$ and defining the m-th *harmonic* number as

$$H_m = \sum_{j=1}^{m}\frac{1}{j}, \tag{9}$$

where $m \in \mathbb{N}$, $m \geq 1$, our starting point is the following

Theorem 1. *Let $x \in (0,2)$. Then*

$$S(x) = -2\gamma_1(1-x) + 2\sum_{k=2}^{+\infty} \frac{\zeta(k)H_{k-1} + \zeta'(k)}{k}(1-x)^k, \tag{10}$$

where γ_1 is defined as in (3)*, H_k is defined as in* (9)*, $\zeta(\cdot)$ is the Riemann zeta-function and $\zeta'(\cdot)$ is its first derivative. Moreover, letting $x \in (0,1) \cup (1,2)$, $n \in \mathbb{N}$, $n \geq 1$ be fixed, and $r_S(x,n) \in \mathbb{N}$,*

$$r_S(x,n) := \left\lceil \frac{(n+2)\log 2 + |\log(1-|1-x|)|}{|\log|1-x||} \right\rceil - 1, \tag{11}$$

we have that there exists $\theta = \theta(x) \in (-0.6, 0.6)$ such that

$$S(x) = -2\gamma_1(1-x) + 2\sum_{k=2}^{r_S(x,n)} \frac{\zeta(k)H_{k-1} + \zeta'(k)}{k}(1-x)^k + |\theta| 2^{-n}. \tag{12}$$

We immediately remark that (10) is the Taylor series centred at 1 of $S(x)$; in particular this implies that

$$S'(1) = 2\gamma_1 \quad \text{and} \quad S^{(k)}(1) = 2(-1)^k(k-1)!\big(\zeta(k)H_{k-1} + \zeta'(k)\big) \quad (k \in \mathbb{N}, k \geq 2).$$

Using Theorem 1 and (1), for $x \in (0,2)$ we trivially have

$$R(x) = -\zeta''(0) + 2(1-x)\gamma_1 - 2\sum_{k=2}^{+\infty} \frac{\zeta(k)H_{k-1} + \zeta'(k)}{k}(1-x)^k$$

and its corresponding truncated version. We remark that (10) is[1] equation (2.14) of Dilcher [5] but we will prove Theorem 1 in a different way, *i.e.*, starting from (5), which in fact reveals that such an argument can be used for any function having an integral representation of Plana's type like the one in (5).

Recalling (4), the fact that Theorem 1 holds for every $x \in (0,2)$ means that every value of $S(x)$, $x \in (0,1)$, can be computed in two different ways.[2] Moreover it is clear that $r_S(x,n)$ becomes larger as $|1-x|$ increases. Hence, recalling that in our applications of Section 4 we are mainly interested in $x \in (0,1)$, if $x \in (1/2, 1)$ we will directly compute $S(x)$ using Theorem 1 while for $x \in (0, 1/2)$ we will shift the problem using (4) and use Theorem 1 in $(1, 3/2)$. In the following we will refer to this procedure as the *shifting trick*. Such an argument leads to the following two corollaries.

Corollary 1. *Let $x \in (0, 1/2)$. We have that*

$$S(x) = (\log x)^2 + 2\gamma_1 x + 2\sum_{k=2}^{+\infty} (-1)^k \frac{\zeta(k)H_{k-1} + \zeta'(k)}{k} x^k. \tag{13}$$

Letting further $n \in \mathbb{N}$, $n \geq 1$ be fixed and $r'_S(x,n) \in \mathbb{N}$,

$$r'_S(x,n) := r_S(1+x,n) = \left\lceil \frac{(n+2)\log 2 + |\log(1-x)|}{|\log x|} \right\rceil - 1,$$

[1] Pay attention to the fact that the Deninger $S(x)$-function defined in (1)-(2) is equal to $-2\log(\Gamma_1(x))$ as defined in Proposition 1 of Dilcher [5].

[2] We remark that the size of the convergence interval of the series in the right hand side of (10) can be doubled by isolating the Taylor series at 1 of $(\log x)^2$ and using the estimates on $|\zeta(n) - 1|$ of Lemma 3 below. We do not insert such an idea here, since the computation of such an extra-factor $(\log x)^2$ leads, in our practical application, to a longer total running time.

where $r_S(u,n)$ *is defined in Theorem* 1*, we have that there exists* $\eta = \eta(x) \in (-0.6, 0.6)$ *such that*

$$S(x) = (\log x)^2 + 2\gamma_1 x + 2 \sum_{k=2}^{r'_S(x,n)} (-1)^k \frac{\zeta(k)H_{k-1} + \zeta'(k)}{k} x^k + \ |\eta| 2^{-n}. \tag{14}$$

Recalling Remark (2.6) of Deninger [3, page 176], (1) and (3) we also obtain

$$S\Big(\frac{1}{2}\Big) = -R\Big(\frac{1}{2}\Big) - \zeta''(0) = \frac{1}{2}(\log \pi)^2 + \frac{\pi^2}{24} - \frac{\gamma_1 + \gamma^2}{2}. \tag{15}$$

Remark 1. As a matter of curiosity, since we are aware of the fact that much faster algorithms exist to compute γ_1, see Johansson-Blagouchine [13], we remark that evaluating twice $S(1/2)$ using Theorem 1 (the first time directly and the second as $S(3/2) + (\log 2)^2$), we have, by subtracting such formulae, that the summands having even indices vanish; thus we obtain

$$\gamma_1 = -\frac{1}{2}(\log 2)^2 + \sum_{\ell=1}^{n/2+1} \frac{\zeta(2\ell+1)H_{2\ell} + \zeta'(2\ell+1)}{(2\ell+1)4^\ell} + 0.6 \cdot 2^{-n}.$$

Such a result, similar to equation (3.10) of Dilcher [5], allows us to fast compute γ_1 with a precision of n bits using about $n/2$ summands. For example, using PARI/GP, we got γ_1 with a precision of 1 000 decimal digits within 1 minute and 34 seconds of computation time on a Dell OptiPlex-3050 machine (equipped with an Intel i5-7500 processor, 3.40GHz, 16 GB of RAM and running Ubuntu 18.04.2).

Combining (12), (14) and (15), we obtain a very fast way of computing $S(x)$ for every $x > 0$. We will see more about this in Section 5 but we also summarise the situation in the following

Corollary 2. *We use the notation introduced in Theorem* 1 *and Corollary* 1*. Moreover, for every* $x > 0$*, we denote as* $\lfloor x \rfloor$ *the integral part of* x *and as* $\{x\} = x - \lfloor x \rfloor$ *the fractional part of* x*. Hence we obtain*:

i) $S(1) = S(2) = 0$ *and* $S(m) = -\sum_{k=2}^{m-1} (\log k)^2$ *for every* $m \in \mathbb{N}$, $m \geq 3$;
ii) *for* $x > 1$, $x \notin \mathbb{N}$, *we compute* $S(x)$ *as* $S(x) = S(\{x\}) - \sum_{k=0}^{\lfloor x \rfloor -1} (\log(\{x\} + k))^2$;
iii) $S(1/2) = (\log \pi)^2/2 + \pi^2/24 - (\gamma_1 + \gamma^2)/2$;
iv) *for* $x \in (0, 1/2)$, *we compute* $S(x)$ *as in* (14);
v) *for* $x \in (1/2, 1)$, *we compute* $S(x)$ *as in* (12).

The proof of Corollary 2 follows just collecting the information coming from Theorem 1, Corollary 1, equations (15) and (4).

Even if in our application we will always work with $x \in (0,1)$, we recall that, for x large, it might be useful to implement the Stirling-like formula proved in Theorem 2.11 of Deninger [3] which gives an asymptotic expression for $R(x)$ and, *a fortiori*, for $S(x)$.

Our second theorem is about the function T defined in (7). As for $S(x)$, the starting point is the following

Theorem 2. *Let* $x \in (0,2)$*. Using the notation introduced in Theorem* 1*, we have*

$$T(x) = \sum_{k=2}^{+\infty} \big(\zeta(k)H_{k-1} + \zeta'(k)\big)(1-x)^{k-1}. \tag{16}$$

Moreover, letting $x \in (0,1) \cup (1,2)$*,* $n \in \mathbb{N}$*,* $n \geq 1$ *be fixed, and* $r_T(x,n) \in \mathbb{N}$*,*

$$r_T(x,n) := \Big\lceil \min_r \Big\{ r \geq 1 + \frac{(n+2)\log 2 - \log|\log|1-x|| + \log\log r}{|\log|1-x||} \Big\} \Big\rceil, \tag{17}$$

we have that there exists $\theta = \theta(x) \in (-1,1)$ *such that*

$$T(x) = \sum_{k=2}^{r_T(x,n)} \big(\zeta(k)H_{k-1} + \zeta'(k)\big)(1-x)^{k-1} \ + \ |\theta| 2^{-n}. \tag{18}$$

We immediately remark that (16) is the Taylor series centred at 1 of $T(x)$; in particular this implies that

$$T^{(k)}(1) = (-1)^k k! \big(\zeta(k+1)H_k + \zeta'(k+1)\big) \quad (k \in \mathbb{N}, k \geq 1).$$

Using Theorem 2 and (7), for $x \in (0,2)$ we trivially have

$$\psi_1(x) = -\gamma_1 + \sum_{k=2}^{+\infty} \big(\zeta(k)H_{k-1} + \zeta'(k)\big)(1-x)^{k-1}$$

and the corresponding truncated version.

Formula (16) is essentially the one in Entry 21(ii) on page 280 of [1] and it follows by differentiation from (10) of Theorem 1. The series in Theorem 2 clearly has a worst convergence speed than the one in Theorem 1 and this justifies the different bound on $r_T(x,n)$ we have in (17) comparing with the one for $r_S(x,n)$ in (11). Recalling (8), the fact that Theorem 2 holds for every $x \in (0,2)$ means that every value of $T(x)$, $x \in (0,1)$, can be computed in two different ways and that the shifting trick can be used in this case too.[3] Hence, if $x \in (1/2,1)$ we will directly compute $T(x)$ using Theorem 2 while for $x \in (0,1/2)$ we will use (8) and Theorem 2 in $(1,3/2)$. This way we obtain the following two corollaries.

Corollary 3. *Let* $x \in (0,1/2)$*. We have that*

$$T(x) = -\frac{\log x}{x} + \sum_{k=2}^{+\infty} (-1)^{k-1} \big(\zeta(k)H_{k-1} + \zeta'(k)\big) x^{k-1}. \tag{19}$$

Letting further $n \in \mathbb{N}$*,* $n \geq 1$ *be fixed and* $r'_T(x,n) \in \mathbb{N}$*,*

$$r'_T(x,n) := r_T(1+x,n) = \Big\lceil \min_r \Big\{ r \geq 1 + \frac{(n+2)\log 2 - \log|\log x| + \log\log r}{|\log x|} \Big\} \Big\rceil,$$

where $r_T(u,n)$ *is defined in Theorem* 2*, we have that there exists* $\eta = \eta(x) \in (-1,1)$ *such that*

$$T(x) = -\frac{\log x}{x} + \sum_{k=2}^{r'_T(x,n)} (-1)^{k-1} \big(\zeta(k)H_{k-1} + \zeta'(k)\big) x^{k-1} \ + \ |\eta| 2^{-n}. \tag{20}$$

Recalling equation (7.14) of Dilcher [4] we also obtain

$$T\Big(\frac{1}{2}\Big) = \gamma_1 + \psi_1\Big(\frac{1}{2}\Big) = (\log 2)^2 + 2\gamma \log 2. \tag{21}$$

[3] We remark that the size of the convergence interval can be doubled by isolating the Taylor series at 1 of $2(\log x)/x$ and using the estimates on $|\zeta(n) - 1|$ of Lemma 3 below. We do not insert such an idea here, since the computation of such an extra-factor $2(\log x)/x$ leads, in our practical application, to a longer total running time.

Remark 2. In this case too we remark that evaluating twice $T(1/2)$ using Theorem 2 (the first time directly and the second as $T(3/2) + 2\log 2$), we have, by summing such formulae, that the summands having even indices vanish; thus we obtain

$$\gamma = -\frac{1}{2}\log 2 + \frac{1}{2} + \frac{1}{2\log 2}\sum_{\ell=1}^{n/2+4} \frac{\zeta(2\ell+1)H_{2\ell} + \zeta'(2\ell+1)}{4^{\ell}} + 2^{-n+1}.$$

Such a result allows us to fast compute γ with a precision of n bits using about $n/2$ steps. For example, using PARI/GP, we got γ with a precision of 1 000 decimal digits within 1 minute and 6 seconds of computation time on the Dell Optiplex machine previously mentioned. In this case too there exist much faster algorithms to perform such a computation, see again [13].

Combining (18), (20) and (21), we obtain a very fast way of computing $T(x)$ for every $x > 0$. We will see more about this in Section 5 but we also summarise the situation in the following

Corollary 4. *We use the notation introduced in Theorem* 2 *and Corollaries* 2-3*. We have*:

i) $T(1) = T(2) = 0$ *and* $T(m) = \sum_{k=2}^{m-1} (\log k)/k$ *for every* $m \in \mathbb{N}$, $m \geq 3$;
ii) *if* $x > 1$, $x \notin \mathbb{N}$, *we compute* $T(x)$ *as* $T(x) = T(\{x\}) + \sum_{k=0}^{\lfloor x \rfloor -1} (\log(\{x\}+k))/(\{x\}+k)$;
iii) $T(1/2) = (\log 2)^2 + 2\gamma \log 2$;
iv) *if* $x \in (0, 1/2)$, *we compute* $T(x)$ *as in* (20);
v) *if* $x \in (1/2, 1)$, *we compute* $T(x)$ *as in* (18).

The proof of Corollary 4 follows just collecting the information coming from Theorem 2, Corollary 3, equations (21) and (8).

We finally remark that the shifting trick applies to any function which can be defined as the solution of a difference equation, like S and T, and that it can be expressed via a power series whose convergence interval is twice as large than the step of the difference equation. Another classical example of such a phenomenon[4] is the pair of functions given by $\log \Gamma$ and $\psi = \Gamma'/\Gamma$, for which the analogues of the formulae (10) and (16) were first proved by Euler, see, *e.g.*, Section 3 of the beautiful survey of Lagarias [15]. But this also holds for further generalisations of Euler's Gamma function like the ones studied by Dilcher in [5]; in fact S and T are the first and easier cases of such generalisations.

Here we are mainly interested in S and T because of the number-theoretic applications concerning the logarithmic derivative at 1 of Dirichlet L-functions, see Section 4. There we will examine how to compute such quantities in a fast way and the number-theoretic consequences we can infer from such data.

The paper is organised as follows: in Sections 2-3 we will respectively prove Theorems 1-2. In Section 4 we will describe the problems in which the use of $S(x)$ and $T(x)$ is relevant. In Section 5 we will discuss the computational costs and some of the implementation features of the formulae in Theorems 1-2 with respect to the applications too. Finally, Section 6 is dedicated to show some figures about the applications described in Section 4.

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2. Proof of Theorem 1

We start with the following lemmas that might have some independent interest too.

[4]We used it in [19] to numerically study Littlewood's bounds on $|L(1,\chi)|$.

Lemma 1. *Let $x > 0$ be fixed, $T(x)$ be defined as in* (7) *and γ_1 as in* (3). *Moreover let γ be the Euler-Mascheroni constant. Then we have*

$$T(x) = \gamma_1 - \int_0^{+\infty} \Big(e^{-t} - \frac{te^{-xt}}{1-e^{-t}}\Big) \frac{\gamma + \log t}{t} \, \mathrm{d}t \tag{22}$$

and

$$\int_0^{+\infty} \Big(e^{-t} - \frac{te^{-t}}{1-e^{-t}}\Big) \frac{\gamma + \log t}{t} \, \mathrm{d}t = \gamma_1. \tag{23}$$

Proof. Using (5) and (8), a differentiation immediately gives (22). The second part follows from the first using $T(1) = 0$. □

Lemma 2. *Let $x > 0$ be fixed, $S(x)$ be defined as in* (2), *$T(x)$ be defined as in* (7) *and γ_1 as in* (3). *Let moreover γ be the Euler-Mascheroni constant. Then we have*

$$T(x) = \int_0^{+\infty} \big(e^{(1-x)t} - 1\big) \frac{\gamma + \log t}{e^t - 1} \, \mathrm{d}t \tag{24}$$

and

$$S(x) = -2(1-x)\gamma_1 + 2\int_0^{+\infty} \big(e^{(1-x)t} - 1 - (1-x)t\big) \frac{\gamma + \log t}{t(e^t - 1)} \, \mathrm{d}t. \tag{25}$$

Proof. Inserting (23) into (22) and performing a trivial computation on absolutely convergent integrals gives (24). Moreover, an algebraic manipulation on equation (5) immediately give

$$\begin{aligned} S(x) = 2\int_0^{+\infty} (x-1)\Big(e^{-t} - \frac{te^{-t}}{1-e^{-t}}\Big) \frac{\gamma + \log t}{t} \, \mathrm{d}t \\ + 2\int_0^{+\infty} \Big(\frac{(x-1)te^{-t} + e^{-xt} - e^{-t}}{1-e^{-t}}\Big) \frac{\gamma + \log t}{t} \, \mathrm{d}t \end{aligned}$$

which is allowed since both integrals absolutely converge. Recalling Lemma 1 we see that the first integral is equal to $2(x-1)\gamma_1$. Another algebraic manipulation on the second integral proves (25). We also remark that (24) can also be obtained by differentiation from (25) and (8). □

We will also need the following elementary estimates.

Lemma 3. *Let γ be the Euler-Mascheroni constant, $\psi(s) = \Gamma'/\Gamma(s)$ be the digamma function and let $x > 0$. Then*

$$\log x - \frac{1}{x} < \psi(x) < \log x.$$

Moreover, for every $k \in \mathbb{N}$, $k \geq 3$, we have $\psi(k) + \gamma = H_{k-1}$,

$$1 < \zeta(k) < 1 + \frac{1}{2^{k-1}} \quad \textit{and} \quad -\frac{3\log 2 + 2}{2^k} < \zeta'(k) < -\frac{\log 2}{2^k}.$$

Proof. The first inequality follows from Theorem 5 of Gordon [8]. The second part follows from (9) and the fact that $\psi(1) = -\gamma$ and $\psi(x+1) = \psi(x) + 1/x$; hence $\psi(k) + \gamma = \sum_{j=1}^{k-1} 1/j$ for every $k \in \mathbb{N}$, $k \geq 2$. The third part of the lemma immediately follows by partial summation from the definition of $\zeta(s)$ and $\zeta'(s)$, $s \in \mathbb{R}$, $s > 1$. □

The proof of Theorem 1 now starts from (25) of Lemma 2. Let $x \in (0, 2)$ and, for every $t \in \mathbb{R}$, define $f(x,t) := e^{(1-x)t} - 1 - (1-x)t$. Hence (25) becomes

$$S(x) = -2(1-x)\gamma_1 + 2\int_0^{+\infty} f(x,t) \frac{\gamma + \log t}{t(e^t - 1)} \, \mathrm{d}t. \tag{26}$$

Writing the Taylor expansion at 0 of $f(x,\cdot)$, we can easily get that $f(x,t) = \sum_{k=2}^{+\infty} t^k(1-x)^k/k!$ which holds for every $t \in \mathbb{R}$ and $x \in (0,2)$. Hence

$$\int_0^{+\infty} f(x,t)\frac{\gamma+\log t}{t(e^t-1)}\,\mathrm{d}t = \sum_{k=2}^{+\infty}\frac{(1-x)^k}{k!}\int_0^{+\infty}\frac{t^{k-1}(\gamma+\log t)}{e^t-1}\,\mathrm{d}t \tag{27}$$

in which we exchanged the series and the integral signs exploiting their absolute convergence. Let now $s \in \mathbb{C}$, $\Re(s) > 1$. Recalling the classical formula

$$\int_0^{+\infty}\frac{t^{s-1}}{e^t-1}\,\mathrm{d}t = \Gamma(s)\zeta(s), \tag{28}$$

differentiating over s we immediately get

$$\int_0^{+\infty}\frac{t^{s-1}\log t}{e^t-1}\,\mathrm{d}t = \Gamma'(s)\zeta(s) + \Gamma(s)\zeta'(s). \tag{29}$$

Recalling that $\psi(s) = \Gamma'/\Gamma(s)$, Lemma 3 and $\Gamma(k) = (k-1)!$, by inserting (28)-(29) into (27) we obtain

$$\int_0^{+\infty} f(x,t)\frac{\gamma+\log t}{t(e^t-1)}\,\mathrm{d}t = \sum_{k=2}^{+\infty}\frac{\zeta(k)H_{k-1}+\zeta'(k)}{k}(1-x)^k. \tag{30}$$

Hence (10) immediately follows by inserting (30) into (26). This proves the first part of Theorem 1. We now prove the second part of Theorem 1. From now on we denote

$$\mathscr{L}(k) := \zeta(k)H_{k-1} + \zeta'(k). \tag{31}$$

Moreover letting $r \in \mathbb{N}$, $r \geq 2$, we define

$$\Sigma_S(r,x) := \sum_{k=2}^{r}\frac{\mathscr{L}(k)}{k}(1-x)^k$$

and $E_S(r,x) := \sum_{k=r+1}^{+\infty}(\mathscr{L}(k)/k)(1-x)^k$. Hence from (10) we get

$$S(x) = -2(1-x)\gamma_1 + 2\Sigma_S(r,x) + 2E_S(r,x). \tag{32}$$

Let now $n \geq 1$ be fixed. For every fixed $x \in (0,2)$, $x \neq 1$, we will find $r = r_S(x,n) \in \mathbb{N}$ such that $|E_S(r,x)| < 0.3 \cdot 2^{-n}$. Using Lemma 3 we obtain, for $k \geq r+1 \geq 3$, that

$$\frac{|\mathscr{L}(k)|}{k} < \frac{\zeta(k)H_{k-1}+|\zeta'(k)|}{k} < \frac{(1+2^{-r})(\log(r+1)+\gamma)+2^{2-r}}{r+1} < 1.04$$

and hence, using the well-known formula about the sum of a geometric progression, we can write

$$|E_S(r,x)| < 1.04\sum_{k=r+1}^{+\infty}|1-x|^k = 1.04\frac{|1-x|^{r+1}}{1-|1-x|}. \tag{33}$$

We now look for $r = r_S(x,n) \in \mathbb{N}$ such that $\frac{|1-x|^{r+1}}{1-|1-x|} \leq 2^{-n-2}$. An easy computation reveals that

$$r+1 \geq \frac{(n+2)\log 2 + |\log(1-|1-x|)|}{|\log|1-x||} \tag{34}$$

suffices. The second part of Theorem 1 then follows from (32)-(34).

3. Proof of Theorem 2

We already remarked that (16) follows via (8) from (10) but a direct proof can also be obtained starting from (24) and arguing as in the proof of Theorem 1. We now prove the second part of Theorem 2. Letting $r \in \mathbb{N}$, $r \geq 2$, and recalling (31), we define

$$\Sigma_T(r, x) := \sum_{k=2}^{r} \mathscr{L}(k)(1-x)^{k-1}$$

and $E_T(r, x) := \sum_{k=r+1}^{+\infty} \mathscr{L}(k)(1-x)^{k-1}$. Hence from (16) we get

$$T(x) = \Sigma_T(r, x) + E_T(r, x). \tag{35}$$

Let now $n \geq 1$ be fixed. For every fixed $x \in (0, 2)$, $x \neq 1$, we will find $r = r_T(x, n) \in \mathbb{N}$ such that $|E_T(r, x)| < 2^{-n}$. Using Lemma 3 we have, for $k \geq r + 1 \geq 4$, that

$$|E_T(r, x)| < \frac{2}{|1-x|} \sum_{k=r+1}^{+\infty} |1-x|^k \log k. \tag{36}$$

Assuming that $r \geq 1/x$, we have that $|1-x|^k \log k$ is a decreasing sequence for $k \geq r+1$; hence a partial integration argument gives that

$$\begin{aligned} |E_T(r, x)| &< \frac{2}{|1-x|} \int_r^{+\infty} |1-x|^u \log u \, \mathrm{d}u < 2\frac{|1-x|^{r-1}}{|\log|1-x||}\Big(\log r + \frac{1}{r|\log|1-x||}\Big) \\ &< 4\frac{|1-x|^{r-1}}{|\log|1-x||} \log r, \end{aligned} \tag{37}$$

in which we also assumed that $r|\log|1-x|| \geq 1$. We now look for $r = r_T(x, n) \in \mathbb{N}$ such that $\frac{|1-x|^{r-1}}{|\log|1-x||} \log r \leq 2^{-n-2}$. An easy computation reveals that

$$r - 1 \geq \frac{(n+2)\log 2 - \log|\log|1-x|| + \log\log r}{|\log|1-x||} \tag{38}$$

suffices. The second part of Theorem 2 then follows from (35)-(38) .

4. Applications

We briefly describe here some number-theoretic applications in which the use of S and T is relevant; we will heavily refer to [17] in which a more detailed presentation is given.

4.1. **Computation of $L'/L(1, \chi)$.** The main application in which is important to know the values of $S(a/q)$ is to evaluate the logarithmic derivative at 1 of the Dirichlet L-functions. Following the line of Section 3 of [17] we have, for χ odd, that

$$\frac{L'}{L}(1, \chi) = \gamma + \log(2\pi) + \frac{1}{B_{1,\overline{\chi}}} \sum_{a=1}^{q-1} \overline{\chi}(a) \log\Big(\Gamma\big(\frac{a}{q}\big)\Big) \tag{39}$$

and, for χ even, $\chi \neq \chi_0$, that

$$\frac{L'}{L}(1, \chi) = \gamma + \log(2\pi) - \frac{1}{2} \frac{\sum_{a=1}^{q-1} \overline{\chi}(a)\, S(a/q)}{\sum_{a=1}^{q-1} \overline{\chi}(a) \log\big(\Gamma(a/q)\big)}, \tag{40}$$

where $B_{1,\chi} := (\sum_{a=1}^{q-1} a\chi(a))/q$ is the first χ-Bernoulli number, $L(s,\chi)$ denote the Dirichlet L-functions, χ run over the non-trivial Dirichlet characters mod q and χ_0 is the trivial Dirichlet character mod q. Using the values of $T(a/q)$ we can alternatively write, for every $\chi \neq \chi_0$, that

$$\frac{L'}{L}(1,\chi) = -\log q - \frac{\sum_{a=1}^{q-1} \chi(a)\, T(a/q)}{\sum_{a=1}^{q-1} \chi(a)\, \psi(a/q)}. \tag{41}$$

The summations over a can be efficiently performed using the Fast Fourier Transform method, see, *e.g.*, Section 4 of [17], and for this approach the use (39)-(40) leads to a faster algorithm than the one which uses (41) because in the former case a *decimation in frequency* strategy can be applied. This essentially means that just the $(q-1)/2$ values of $S(a/q) + S(1-a/q)$ are needed to perform the summation over a in (40); combining this with the use of suitable reflection formulae for $S(x)$ lead to gain a factor 4 in the computational cost of generating the S-values with respect to the cost of generating the T-values, see also subsection 5.3.

It is a well-known fact that the size of the logarithmic derivative at 1 of the Dirichlet L-functions is connected with the horizontal distribution of non-trivial zeros of $L(s,\chi)$. In particular it is interesting to study their extremal values under the assumption of the Generalised Riemann Hypothesis.

4.2. **Extremal values of $L'/L(1,\chi)$.** For every odd prime q we define

$$M_q^{\mathrm{odd}} := \max_{\chi \text{ odd}} \left|\frac{L'}{L}(1,\chi)\right|, \quad M_q^{\mathrm{even}} := \max_{\substack{\chi\neq\chi_0\\ \chi \text{ even}}} \left|\frac{L'}{L}(1,\chi)\right|, \quad M_q = \max_{\chi\neq\chi_0} \left|\frac{L'}{L}(1,\chi)\right|.$$

Hence we can compute $M_q = \max(M_q^{\mathrm{odd}}, M_q^{\mathrm{even}})$ using (39)-(40). Numerical values for M_q were obtained in [17] for every odd prime $q \le 10^6$. Such data are in agreement with the estimate proved by Ihara-Murty-Shimura [12] (please remark that our M_q is denoted as Q_m there) since they proved that $M_q \le (2 + o(1)) \log\log q$ as q tends to infinity, under the assumption of the Generalised Riemann Hypothesis. On the other hand, Lamzouri, in a personal communication with the first author, remarked that, by adapting the techniques in his paper [16], one can show that if q is a large prime then $M_q \ge (1 + o(1)) \log\log q$.

We will extend here the study of M_q to the larger interval $q \le 10^7$; we can do so because of the much faster algorithm to compute $S(a/q)$ presented here.

4.3. **The Euler-Kronecker constants for prime cyclotomic fields.** Let q be an odd prime, ζ_q be a primitive q-root of unity, $\zeta_{\mathbb{Q}(\zeta_q)}(s)$ be the Dedekind zeta-function of $\mathbb{Q}(\zeta_q)$. It is a well known fact that $\zeta_{\mathbb{Q}(\zeta_q)}(s)$ has a simple pole at $s = 1$; writing the expansion of $\zeta_{\mathbb{Q}(\zeta_q)}(s)$ near $s = 1$ as

$$\zeta_{\mathbb{Q}(\zeta_q)}(s) = \frac{c_{-1}}{s-1} + c_0 + \mathcal{O}(s-1),$$

the *Euler-Kronecker constant of* $\mathbb{Q}(\zeta_q)$ is defined as

$$\lim_{s\to1}\Big(\frac{\zeta_{\mathbb{Q}(\zeta_q)}(s)}{c_1} - \frac{1}{s-1}\Big) = \frac{c_0}{c_{-1}}.$$

In this cyclotomic case we have that the Dedekind zeta-function can be written as $\zeta_{\mathbb{Q}(\zeta_q)}(s) = \zeta(s)\prod_{\chi\neq\chi_0} L(s,\chi)$, where $\zeta(s)$ is the Riemann zeta-function. By logarithmic differentiation, we immediately get that the *Euler-Kronecker constant for the prime cyclotomic field* $\mathbb{Q}(\zeta_q)$ is

$$\mathfrak{G}_q := \gamma + \sum_{\chi\neq\chi_0} \frac{L'}{L}(1,\chi).$$

Sometimes the quantity $\mathfrak{G}_q$ is denoted as γ_q but this conflicts with notations used in literature. Another interesting quantity related to $\mathfrak{G}_q$ is the Euler-Kronecker constant $\mathfrak{G}_q^+$ for $\mathbb{Q}(\zeta_q + \zeta_q^{-1})$, the maximal real subfield of $\mathbb{Q}(\zeta_q)$. According to eq. (10) of Moree [20] it is defined as

$$\mathfrak{G}_q^+ := \gamma + \sum_{\substack{\chi \neq \chi_0 \\ \chi \text{ even}}} \frac{L'}{L}(1, \chi).$$

An extensive study about the properties of $\mathfrak{G}_q$ and $\mathfrak{G}_q^+$ was recently started by Ihara [10, 11] and carried over from many others; we just recall here the papers by Ford-Luca-Moree [6] and Languasco [17] because they both have some computational results on $\mathfrak{G}_q$ and $\mathfrak{G}_q^+$.

For both $\mathfrak{G}_q$ and $\mathfrak{G}_q^+$ it is interesting to find their negative values since Ihara conjectured that both these quantities should be positive. Such a conjecture for $\mathfrak{G}_q$ was disproved by Ford-Luca-Moree [6] (other two occurrences of $\mathfrak{G}_q < 0$ were detected in [17]). No negative values of $\mathfrak{G}_q^+$ are known so far. We will extend here the search for negative values of $\mathfrak{G}_q$ and $\mathfrak{G}_q^+$ to the larger bound $q \leq 10^7$; in this way we also prove that there are no negative values for both $\mathfrak{G}_q$ and $\mathfrak{G}_q^+$ for every odd prime q up to 10^7. We also evaluate such quantities for some very large q. We can do so because of the much faster algorithm to compute $S(a/q)$ presented here.

5. Implementation

We discuss here some implementation features of the formulae in Corollaries 2 and 4. Since for $x > 1$ we can reduce the problem of evaluating $S(x)$, or $T(x)$, to a sum of a finite number of log-values plus $S(\{x\})$, or $T(\{x\})$, in this Section we assume that $x \in (0, 1)$.

5.1. **Number of summands.** We already remarked in the Introduction that, from the estimates on $r_S(x, n)$ and $r_T(x, n)$ in Theorems 1-2, the number of needed terms we have to consider to have a n-bits digit precision result becomes arbitrarily large as $x \to 0^+$. To avoid this problem we can in practice use the formulae in Corollaries 2 and 4. In both corollaries it is clear that the worst cases for $r_S(x, n)$ and $r'_S(x, n)$ (and, respectively, for $r_T(x, n)$ and $r'_T(x, n)$) are obtained when x approaches $1/2$. Hence we can get any value of $S(x)$, $x \in (0, 1)$, with a precision of n binary digits, with at most $n + 2$ summands (assuming that the needed log and $\mathscr{L}(k)$ values can be obtained with the same precision). Analogously we can get any value of $T(x)$, $x \in (0, 1)$, with a precision of n binary digits, with at most $n + 4 + \log\log(n + 4)$ summands (assuming that the needed log and $\mathscr{L}(k)$ values can be obtained with the same precision).

5.2. **Precomputed coefficients.** In (12) and (18) we have a power series whose coefficients involve the values $\mathscr{L}(k)$, $k \in \mathbb{N}$, $k \geq 2$ (see (31) for the definition of $\mathscr{L}(k)$). Hence in both cases such values can be precomputed, stored and reused for any $x \in (0, 1)$. Moreover, the estimates in Lemma 3 imply that $|\zeta(k) - 1| < 10^{-200}$ for $k \geq 160$ and $|\zeta'(k)| < 10^{-200}$ for $k \geq 420$. Hence, after about 420 terms just the contribution of H_{k-1} matters in (12) and (18). So, after few hundreds terms, the problem of obtaining $\mathscr{L}(k)$ reduces to being able to evaluate H_{k-1}. We also remark that the computation of the needed first hundreds values of $\zeta(k)$ and $\zeta'(k)$ can be performed, for instance, using PARI/GP.

Another nice aspect we have in (12) and (18) is that the powers $(1 - x)^k$ can be computed by recurrence, starting from $(1 - x)^2$ and $1 - x$, respectively. The same clearly holds for equations (14) and (20) too.

All these remarks also reveal that the tasks of evaluating $S(x)$ and $T(x)$ are essentially as difficult as evaluating $(\log x)^2$ and $(\log x)/x$, when x is close to 0.

5.3. **Reflection formulae for** $S(x)$**.** As mentioned in Section 4.1 and extensively explained in Section 4 of [17], the use of the FFT algorithm is important to efficiently compute $\mathfrak{G}_q$, $\mathfrak{G}_q^+$ and M_q. In particular, using $S(x)$, a decimation in frequency strategy can be implemented and hence it is important to have the following *reflection formulae* for S.

We directly express such formulae using Theorem 1 and Corollary 1, or Corollary 2, even if similar ones which use (2) and (5) are also available (such formulae were in fact used in [17], see Section 4.2 there).

Proposition 1. *Let* $x \in (0,1)$*,* $x \neq 1/2$*,* $n \in \mathbb{N}$*,* $n \geq 2$*,* $r_1(x,n) = \lceil \frac{(n+2)\log 2 + |\log(1-x)|}{|\log x|} - 1\rceil/2$ *and* $r_2(x,n) = \lceil \frac{(n+2)\log 2 + |\log x|}{|\log(1-x)|} - 1\rceil/2$*. Using* (31) *and the notations of Theorem* 1 *and Corollary* 2*, we have that there exists* $\theta = \theta(x)$ *such that*

$$S(x) + S(1-x) = (\log x)^2 + 2\sum_{\ell=1}^{r_1} \frac{\mathcal{L}(2\ell)}{\ell} x^{2\ell} + |\theta| 2^{-n}, \quad \big(0 < x < \frac{1}{2}\big), \tag{42}$$

and

$$S(x) + S(1-x) = (\log(1-x))^2 + 2\sum_{\ell=1}^{r_2} \frac{\mathcal{L}(2\ell)}{\ell} (1-x)^{2\ell} + |\theta| 2^{-n}, \quad \big(\frac{1}{2} < x < 1\big). \tag{43}$$

Proof. Assume that $0 < x < 1/2$; in this case we compute $S(x)$ with (13) and $S(1-x)$ with (10). Since the series absolutely converge, their sum is the series having as summands the sum of their coefficients. Arguing as in (33), remarking that $r_1(x,n) = r_S(1-x,n)/2 = r'_S(x,n)/2$ and recalling (31), we immediately have that (42) holds since the odd summands vanish. Assume that $1/2 < x < 1$; in this case we compute $S(x)$ with (10) and $S(1-x)$ with (13). Arguing as for $x \in (0,1/2)$, remarking that $r_2(x,n) = r_S(x,n)/2 = r'_S(1-x,n)/2$ and recalling (31), we immediately have that (43) holds since the odd summands vanish. This completes the proof. □

The corresponding series for (42)-(43) are

$$S(x) + S(1-x) = (\log x)^2 + 2\sum_{\ell=1}^{+\infty} \frac{\mathcal{L}(2\ell)}{\ell} x^{2\ell} \quad \big(0 < x < \frac{1}{2}\big), \tag{44}$$

$$S(x) + S(1-x) = (\log(1-x))^2 + 2\sum_{\ell=1}^{+\infty} \frac{\mathcal{L}(2\ell)}{\ell} (1-x)^{2\ell} \quad \big(\frac{1}{2} < x < 1\big). \tag{45}$$

We remark that in Proposition 1 we have $r_2(x,n) = r_1(1-x,n)$ for $x \in (0,1)$ and hence the right hand side of (43) can be obtained from the the right hand side of (42) just replacing any occurrence of x with $1-x$ and viceversa. Analogous formulae, involving just the odd summands, can also be obtained for $S(x) - S(1-x)$ but we omit them since they have no use in the applications here considered.

The use of Proposition 1 in our application is four times faster than using (18) and (19) for the following reasons:

- exploiting the decimation in frequency strategy we just need to evaluate (42)-(43) at $x = a/q$, for every $a = 1, \ldots, (q-1)/2$, while (18) and (19) need to be evaluated for every $a = 1, \ldots, q-1$. This improves the computational cost of a factor 2;
- the cancellation of the odd terms we have in (42)-(43) leads to another gain of a factor 2 in the computational cost with respect to (18) and (19) since we just need to use half of the summands (the ones with even indices);

- in (42)-(43) the values of the Riemann ζ-function at even integers are required and for them we can use the well-known exact formulae involving the Bernoulli numbers B_k: $\zeta(2\ell) = (-1)^{\ell+1}\frac{B_{2\ell}(2\pi)^{2\ell}}{2(2\ell)!}$, for every $\ell \in \mathbb{N}$, $\ell \geq 1$, where the Bernoulli numbers B_k are defined using the following series expansion: $\frac{t}{e^t-1} = \sum_{k=0}^{+\infty} B_k \frac{t^k}{k!}$, $|t| < 2\pi$, see, *e.g.*, Cohen's book [2, chapter 9].

As we said before, the use of Proposition 1, if possible, is particularly efficient. To compare the practical running times of using (42)-(43) with previous implementations, which used the series/integral definitions of $S(x)$, see (2) and (5), we compared the two PARI/GP scripts used to obtain $S(a/q) + S(1 - a/q)$ for every $a = 1, \dots, (q-1)/2$ when $q = 305741$, 6766811, 212634221. The gain in speed is huge, and it seems to improve as q becomes larger: we observed that the use of (42)-(43) leads to a computation time for $S(a/q) + S(1-a/q)$ (with a precision of 128 bits) for every $a = 1, \dots, (q-1)/2$ which is respectively about 405, 829, 1206 times faster for the three primes mentioned before.

Further practical experiments confirmed such a computational time gain; we will see more on this in the next subsections.

5.4. **Computational costs for the problems of Section 4.** The applications described in Section 4 require to evaluate (12) over $x = a/q$, $a = 1, \dots, q-1$. Using the estimates in subsection 5.1 we have $r_S(x, n), r'_S(x, n) \leq n + 2$ for every $x \in (1/2, 1)$ and, respectively, $x \in (0, 1/2)$. Hence the total cost of evaluating (12) over $x = a/q$, for every $a = 1, \dots, q-1$, is $\mathfrak{O}(qn)$ floating point products, with a precision of n binary digits, and $\mathfrak{O}(q)$ evaluation of the logarithm function at rational points less than $1/2$. Since the remaining part of the computations in our applications are three Fourier Transforms of length $\leq q-1$, see [17, Table 1], having a cost of $\mathfrak{O}(q\log q)$ floating point products each, this proves that the total computational cost of our applications is $\mathfrak{O}(q(n + \log q))$ floating point products, with a precision of n binary digits. In practice, since in such applications we can use a decimation in frequency strategy, Proposition 1 let us directly evaluate $S(a/q) + S(1 - a/q)$ for every $a = 1, \dots, (q-1)/2$ thus reducing of a factor at least 4 the cost of such a step. A similar asymptotic estimate $\mathfrak{O}(q(n + \log q))$ holds also using (18) in the applications but in this case we cannot use the decimation in frequency strategy, see again [17]; hence in practice such an algorithm has a total cost which is about four times larger than the one which uses the S-function. Anyway, we will need such a T-function implementation to double check particularly important results, for example the ones about the negativity of the Euler-Kronecker constant $\mathfrak{G}_q$.

5.5. **Actual implementation of the S and T formulae.** Using the C programming language, we implemented the formulae of Proposition 1 since they are the ones needed for the applications of Section 4. The summation is performed combining the "pairwise summation" [9] algorithm with Kahan's [14] method (the minimal block for the pairwise summation algorithm is summed using Kahan's method) to have a good compromise between precision, computational cost and execution speed. To write here a practical computation time, we remark that for $q = 50\,040\,955\,631$ such an implementation computed $S(a/q) + S(1-a/q)$ for every $a = 1, \dots, (q-1)/2$ with a precision of 128 bits in about nine hours using a single computing core of an HP machine equipped with 4 x Eight-Core Intel(R) Xeon(R) CPU E5-4640 0 @ 2.40GHz, and 256GB of RAM. For comparison, in this case the expected running time of the implementation used in [17] would be about 3475 days on the same machine mentioned before (about 9350 times slower).

Clearly this huge improvement let us evaluate the quantities described in Section 4 for some really large prime numbers and also to extend their knowledge for every odd prime up to 10^7.

Moreover, to be able to double check the results obtained with the S-function, we analogously implemented the formulae of Corollary 4.

5.6. **FFT implementation and computational results.** To implement the FFT method we used the FFTW [7] package which is also able to handle very large cases via its `guru64` interface. Moreover, to be able to store the large arrays of data we produce to initialise the input sequences involved in the FFT and their outputs, we used the `mmap` UNIX system call to map such arrays on the hard disk instead of storing them on the RAM during the execution of the C-programs. Thus we were able to enlarge the range of possible computations we can perform far beyond the size of the available RAM memory. But that was not enough to handle a large case we would like to evaluate: $q = 50\,040\,955\,631 = 2 \cdot 5 \cdot 5\,004\,095\,563 + 1$. We have chosen this prime number because its evaluation using the function $v(q)$, defined in the next paragraph, see (47), is "large" enough to let us think that it might be a good canditate to have $\mathfrak{G}_q < 0$ ($v(50040955631) = 1.2194\dots$); please see the next paragraph for more about $v(q)$ and its link with the negativity of $\mathfrak{G}_q$. Moreover, analysing the prime factor structure of the known examples for which $\mathfrak{G}_q$ is negative, namely $q = 964477901, 9109334831, 9854964401$, see [6] and [17], we see that such primes q have all a "large" prime in the factorisation of $q-1$: $964\,477\,901 = 2 \cdot 5 \cdot 9\,644\,779 + 1$, $9\,109\,334\,831 = 2 \cdot 5 \cdot 910\,933\,483 + 1$, $9\,854\,964\,401 = 2^4 \cdot 5^2 \cdot 197 \cdot 125\,063 + 1$. These two motivations are hence a strong suggestion about the negativity of $\mathfrak{G}_{50040955631}$, even if they are not sufficient to be certain of this.

The presence of a "large" prime factor in the factorisation of $q-1$ leads in fact to another problem in using the so-called `plan-generation` step of the FFTW package. The `plan-generation` step of FFTW is a procedure in which FFTW self-decides how to combine several FFT algorithms to obtain their best combination to solve the particular instance of the problem the user is interested in. This procedure also depends on the prime factorisation of the length of the transform N: in our case $N = q - 1$, or $N = (q - 1)/2$. When N has at least one "large" prime factor, as in our case, the plan-generation step might be very demanding in term of memory usage (RAM). To overcome this, we have then to insert the use of `mmap` in the body of the FFTW code to be able to divert the memory usage of the `plan-generation` step from the RAM to the hard disk. Clearly this increases the actual computation time but, at the same time, let us handle much larger cases, since, essentially, it is much easier, and cheaper, to retrieve large hard disks than a large quantity of RAM.

In this way we obtained a program that needed at most 128GB of RAM at runtime and we used it to perform the computation for the case of $q = 50\,040\,955\,631$ on the University of Padova Strategic Research Infrastructure "CAPRI" (Intel(R) Xeon(R) Gold 6130 CPU @ 2.10GHz, with 256 cores and equipped with 6TB of RAM). The total hard disk usage was about 3.2TB, the time needed for one computing core to generate the S-values with a precision of 128 bits was about six hours and 6 minutes, the `plan-generation` step required about four hours and 5 minutes and the actual FFT transforms about 2 days and half (for S). The total computation time was about two weeks; we recall that such computation times are affected, as above remarked, from the fact that we were using a slower memory device (the hard disk is used instead of RAM). We got that $\mathfrak{G}_{50040955631} = -0.16595399\dots$ and $\mathfrak{G}^+_{50040955631} = 13.89764738\dots$ thus getting another occurrence of a negative Euler-Kronecker constant.

The computation of $\mathfrak{G}_q, \mathfrak{G}_q^+$ and M_q for every odd prime q up to 10^7 was performed on CAPRI using at most 60 computing nodes and it required about 48 hours of time (the global execution time, obtained by summing the declared computing time on each node, was of 101 days and 6 hours).

In this range we obtained that there are no negative values for both $\mathfrak{G}_q$ and $\mathfrak{G}_q^+$ and that

$$\frac{17}{20}\log\log q < M_q < \frac{5}{4}\log\log q \tag{46}$$

for every odd prime $1531 < q \le 10^7$. Moreover the lower bound in (46) holds true for $q > 13$.

The programs used and the results here described are collected at the following address `http://www.math.unipd.it/~languasc/Scomp-appl.html`.

6. Figures

We give here some comments about Figures 1-5 and discuss the role of the $\nu(q)$-function.

Referring to Section 4.5 of [17], we recall the definition of $\mathcal{B}$, the "greedy sequence of prime offsets", `http://oeis.org/A135311`. We define $\mathcal{B}$ using induction, by $b(1) = 0 \in \mathcal{B}$ and $b(n) \in \mathcal{B}$ if it is the smallest integer exceeding $b(n-1)$ such that for every prime r the set $\{b(i) \bmod r\colon 1 \le i \le n\}$ has at most $r-1$ elements. Let now

$$m(\mathcal{A}) := \sum_{i=1}^{s} \frac{1}{a_i},$$

where $\mathcal{A}$ is an admissible set, *i.e.*, $\mathcal{A} = \{a_1, \dots, a_s\}$, $a_i \in \mathbb{N}$, $a_i \ge 1$, such that does not exist a prime p such that $p \mid n\prod_{i=1}^{s}(a_i n + 1)$ for every $n \ge 1$. Thanks to Theorem 2 of Moree [20], if the prime k-tuples conjecture holds and if $\mathcal{A}$ is an admissible set, then $\mathfrak{G}_q < (2 - m(\mathcal{A}) + o(1))\log q$ for $\gg x/(\log x)^{-|\mathcal{A}|-1}$ primes $q \le x$. Moreover, by Theorem 6 of Moree [20], assuming both the Elliott-Halberstam and the prime k-tuples conjectures, if $\mathcal{A}$ is an admissible set then $\mathfrak{G}_q = (1 - m(\mathcal{A}) + o(1))\log q$ for $\gg x/(\log x)^{-|\mathcal{A}|-1}$ primes $q \le x$. We recall that the greedy sequence of prime offsets $\mathcal{B}$ has the property that any finite subsequence is an admissible set. With a PARI/GP script we computed the first 2089 elements of $\mathcal{B}$ since for $\mathcal{C} := \{b(2), \dots, b(2089)\}$ we get $m(\mathcal{C}) > 2$.

So, if we are looking for negative values of $\mathfrak{G}_q$, it seems to be a good criterion to evaluate $\mathfrak{G}_q$ for a prime number q such that $bq + 1$ is prime for many elements $b \in \mathcal{C}$ (clearly it is better to start with the smaller available b's). To be able to measure this fact, we define

$$\nu(q) := \sum_{\substack{2 \le i \le 2089;\ b(i)\in\mathcal{C} \\ b(i)q+1 \text{ is prime}}} \frac{1}{b(i)} \tag{47}$$

and we use such a function to classify $\mathfrak{G}_q$ and $\mathfrak{G}_q^+$ in the following way. In the scatter plots of Figures 1-2 we classified the normalised values of $\mathfrak{G}_q$ and $\mathfrak{G}_q^+$ according to $\nu(q)$. Orange points are the more frequent ones (72.88% of the total number) and satisfy $\nu(q) \le 0.25$; green points satisfy $0.25 < \nu(q) \le 0.5$ (18.29%); blue points satisfy $0.5 < \nu(q) \le 0.75$ (5.98%); black points satisfy $0.75 < \nu(q) \le 1$ (2.77%); red points satisfy $\nu(q) > 1$ (0.08%). The behaviour of $\mathfrak{G}_q$ is the expected one since the red strip essentially corresponds with its minimal values, while the minima of $\mathfrak{G}_q^+$ seem to be less related to $\nu(q)$; we plan to investigate this phenomenon in the next future.

In Figures 3-5 we present the scatter plots on M_q and $M'_q := M_q/\log\log q$. All the plots were obtained using GNUPLOT, v.5.2, patchlevel 8.

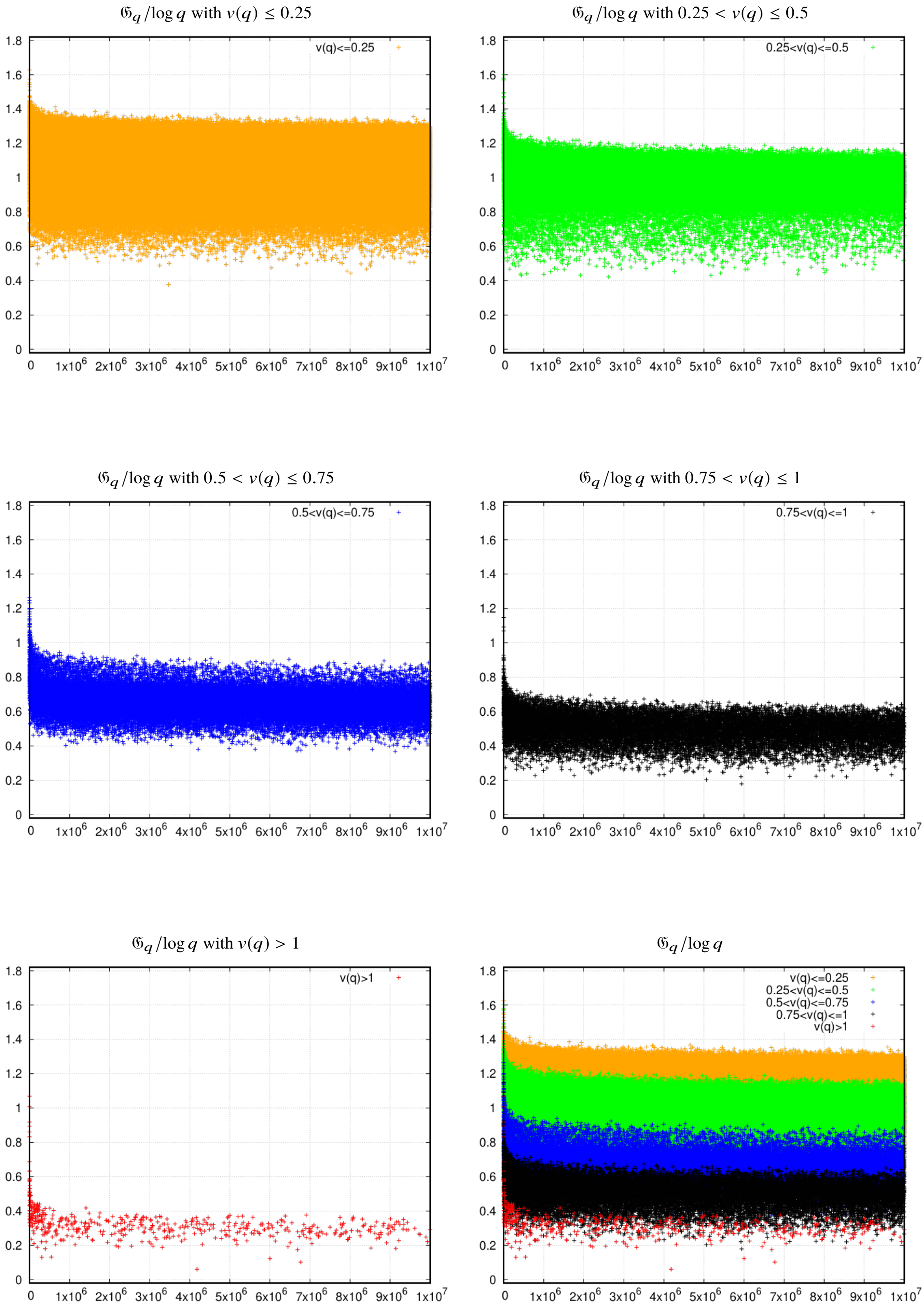

FIGURE 1. The values of $\mathfrak{S}_q/\log q$, q prime, $3 \le q \le 10^7$, classified using $v(q)$. The minimal value is $0.060532\ldots$ and it is attained at $q = 4178771$; the maximal value is $1.626934\ldots$ and it is attained at $q = 19$.

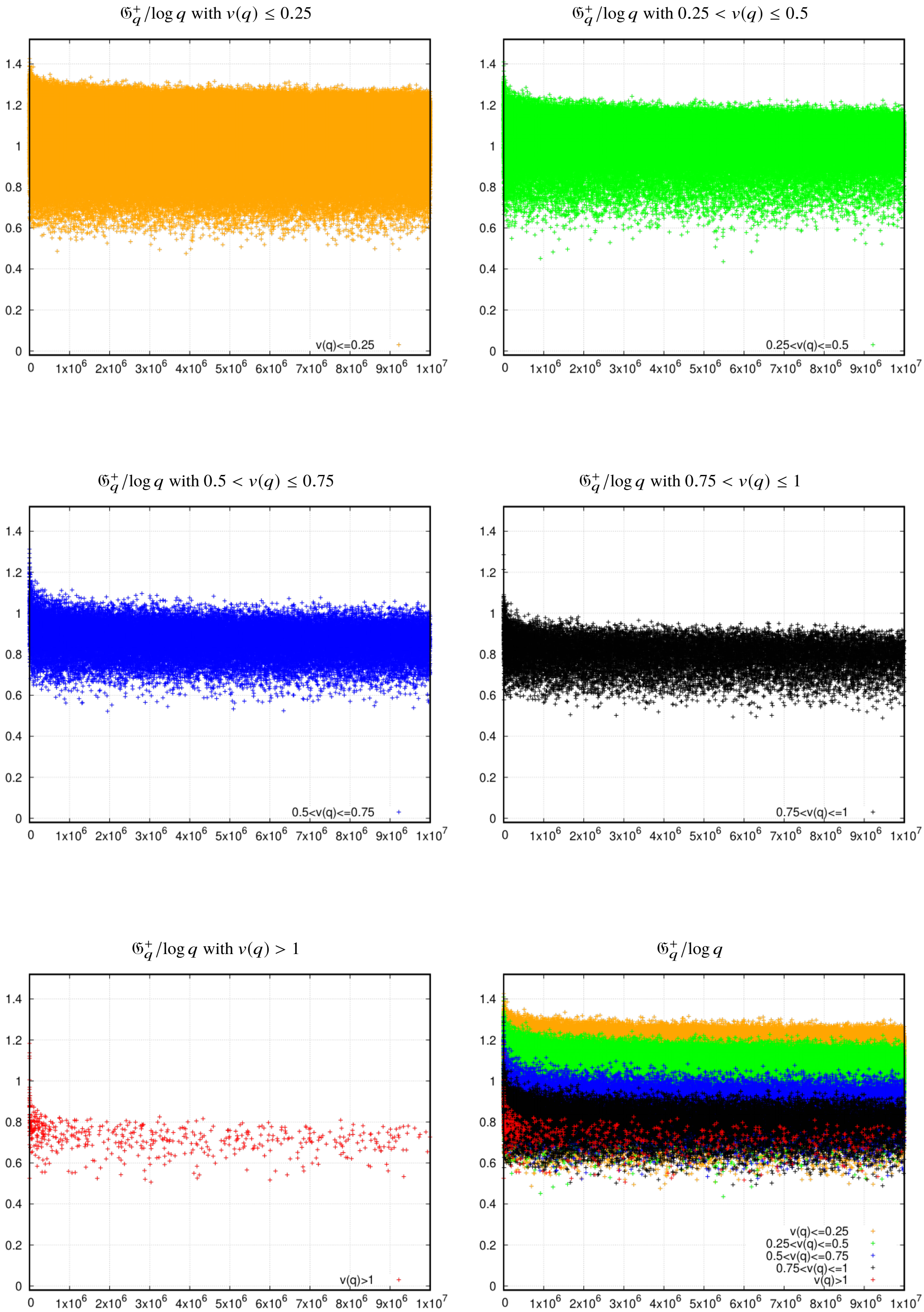

FIGURE 2. The values of $\mathfrak{G}_q^+/\log q$, q prime, $3 \le q \le 10^7$, classified using $v(q)$. The minimal value is $0.436031\ldots$ and it is attained at $q = 5483977$; the maximal value is $1.426263\ldots$ and it is attained at $q = 2053$.

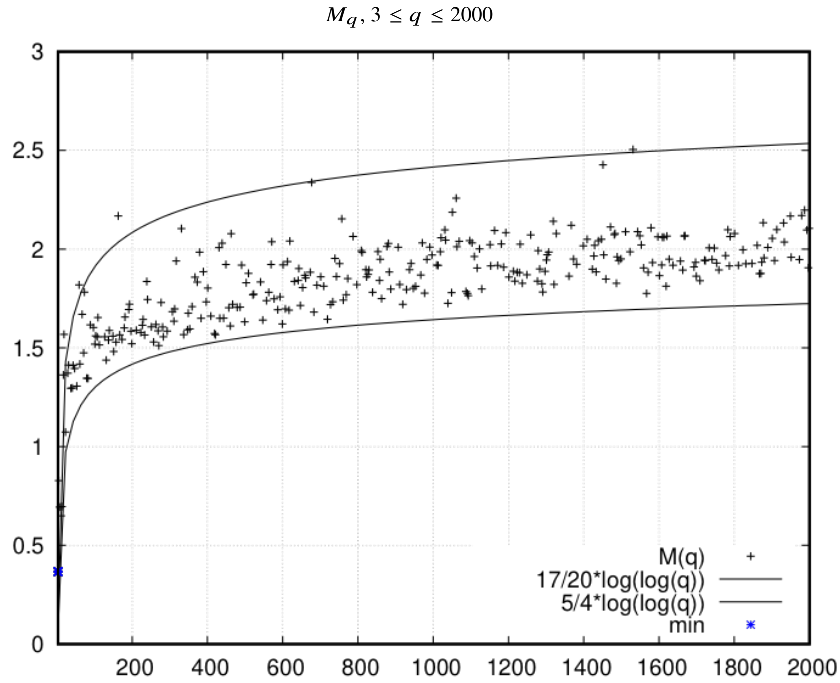

Figure 3. The values of M_q, q prime, $2000 < q \le 10^7$. The minimal value is $0.3682816\ldots$ and it is attained at $q = 3$. The lines represent the functions $c \cdot \log\log q$, with $c = 17/20$ and $c = 5/4$.

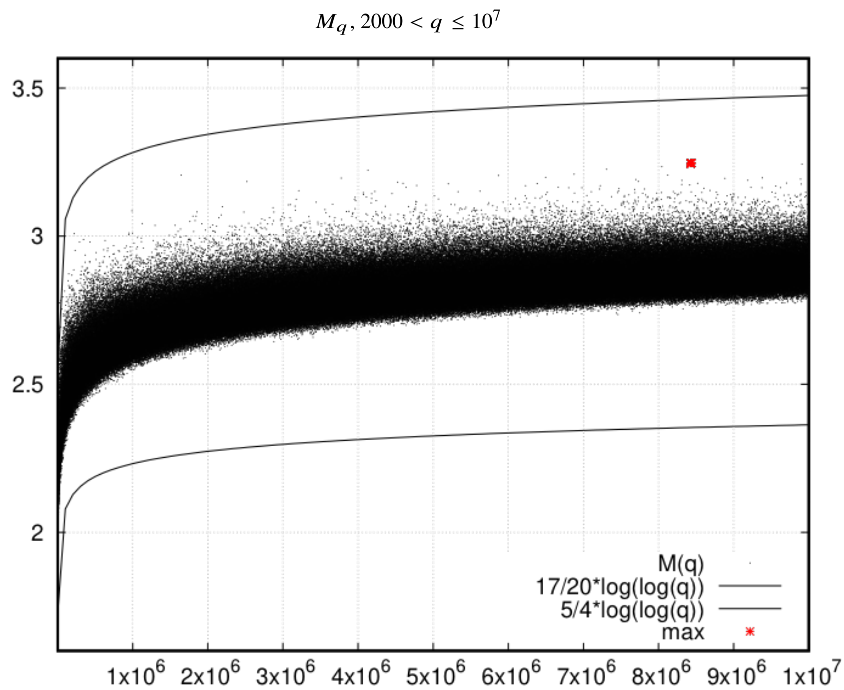

Figure 4. The values of M_q, q prime, $2000 < q \le 10^7$. The maximal value is $3.2466918\ldots$ and it is attained at $q = 8430391$. The lines represent the functions $c \cdot \log\log q$, with $c = 17/20$ and $c = 5/4$.

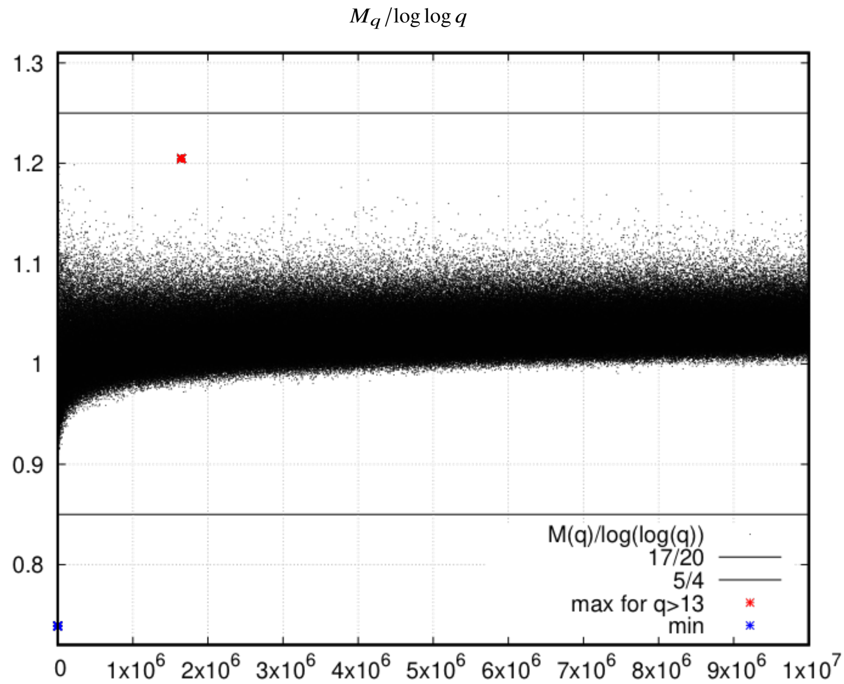

FIGURE 5. The values of $M'_q := M_q/\log\log q$, q prime, $3 \le q \le 10^7$. The minimal value is $0.7392305\ldots$ and it is attained at $q = 13$; the maximal value is $3.9158971\ldots$ and it is attained at $q = 3$ (not represented in the plot); the maximal value for every $q > 13$ is $1.204704\ldots$ and it is attained at $q = 1645093$. The lines represent the constant functions $c = 17/20$ and $c = 5/4$.

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