Computing the Mertens and Meissel–Mertens Constants for Sums over Arithmetic Progressions

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with an Appendix by Karl K. Norton

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We give explicit numerical values with 100 decimal digits for the Mertens constant involved in the asymptotic formula for $\sum_{\substack{p\le x\\ p\equiv a \bmod q}} 1/p$ and, as a byproduct, for the Meissel–Mertens constant defined as $\sum_{p\equiv a \bmod q}(\log(1-1/p)+1/p)$, for $q \in \{3,\dots,100\}$ and $(q,a)=1$. The complete set of results is available online (http://www.math.unipd.it/~languasc/Mertens-comput.html).

1. INTRODUCTION

In this paper we use the technique developed in [Languasco and Zaccagnini 09] to compute the constants $M(q,a)$ involved in the following asymptotic formula:

$$\sum_{\substack{p\le x\\ p\equiv a \bmod q}} \frac{1}{p} = \frac{\log\log x}{\varphi(q)} + M(q,a) + \mathcal{O}_q\left(\frac{1}{\log x}\right), \quad (1\text{–}1)$$

where $x \to +\infty$, and the Meissel–Mertens constant $B(q,a)$ is defined as

$$B(q,a) := \sum_{p\equiv a \bmod q} \left(\log\left(1-\frac{1}{p}\right)+\frac{1}{p}\right),$$

where, here and throughout the present paper, $q\ge 3$ and a are fixed integers with $(q,a)=1$, p denotes a prime number, and $\varphi(q)$ is the usual Euler totient function.

In fact, we will see how to compute $M(q,a)$ with a precision of 100 decimal digits, and we will use the results in [Languasco and Zaccagnini 09] to obtain well-approximated values for $B(q,a)$.

To do so, we recall that the constant $C(q,a)$ studied in [Languasco and Zaccagnini 07, Languasco and Zaccagnini 09] is defined implicitly by

$$P(x;q,a) := \prod_{\substack{p\le x\\ p\equiv a \bmod q}} \left(1-\frac{1}{p}\right) = \frac{C(q,a)}{(\log x)^{1/\varphi(q)}}(1+o(1)) \quad (1\text{–}2)$$

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as $x \to +\infty$. In [Languasco and Zaccagnini 07], we proved that

$$C(q,a)^{\varphi(q)} = e^{-\gamma} \prod_p \left(1 - \frac{1}{p}\right)^{\alpha(p;q,a)},$$

where $\alpha(p;q,a) = \varphi(q) - 1$ if $p \equiv a \bmod q$ and $\alpha(p;q,a) = -1$ otherwise, and γ is the Euler constant. This enabled us to compute their values to 100 decimal digits in [Languasco and Zaccagnini 09].

Taking the logarithm of both sides in (1–2), we get that

$$\sum_{\substack{p \le x \\ p \equiv a \bmod q}} \log\left(1 - \frac{1}{p}\right) = \log C(q,a) - \frac{\log\log x}{\varphi(q)} + o(1)$$

as $x \to +\infty$, and hence, adding (1–1), we obtain

$$M(q,a) = B(q,a) - \log C(q,a). \tag{1–3}$$

By (1–3) and using the results in [Languasco and Zaccagnini 09] together with the computation of $M(q,a)$ that we will explain below, we can compute the corresponding values for $B(q,a)$ in the same range (and with the same precision) for any $q \in \{3,\dots,100\}$ and $(q,a) = 1$.

We recall that $M(q,a)$ and $C(q,a)$ were computed in [Finch 07] in the case $q \in \{3,4\}$ and $(q,a) = 1$. For more information on the literature about these (and many other) constants, we suggest that the reader have a look at [Finch 03].

The referee of this paper and Robert Baillie [Baillie 09] independently remarked that a computation similar to ours with q up to 10000 suggests that

1. as $q \to \infty$, $M(q,1)$ approaches 0,
2. as $q \to \infty$, $M(q,2)$ approaches $1/2$,

and asked whether this is actually true. This in fact follows from the following result by Karl K. Norton [Norton 09]: If $1 \le a < q$, then

$$\lim_{\substack{q \to +\infty \\ (q,a)=1}} M(q,a) = \begin{cases} 1/a & \text{if } a \text{ is a prime number,} \\ 0 & \text{otherwise,} \end{cases} \tag{1–4}$$

and the limit is uniform on a. We will see how to prove (1–4) in §4.

2. THEORETICAL FRAMEWORK

From now on, we will let χ be a Dirichlet character modulo q. By the orthogonality of Dirichlet characters, a direct computation and [Hardy and Wright 79, Theorem 428] show that

$$\varphi(q) M(q,a) = \gamma + B - \sum_{p \mid q} \frac{1}{p} + \sum_{\substack{\chi \bmod q \\ \chi \ne \chi_0}} \overline{\chi}(a) \sum_p \frac{\chi(p)}{p}, \tag{2–1}$$

where

$$B := \sum_p \left(\log\left(1 - \frac{1}{p}\right) + \frac{1}{p}\right) \tag{2–2}$$

is the Meissel–Mertens constant.

Moreover, using the Taylor expansion of $\log(1-x)$ and again by orthogonality, it is clear that

$$\begin{aligned} \varphi(q) B(q,a) &= -\sum_{\chi \bmod q} \overline{\chi}(a) \sum_{m \ge 2} \frac{1}{m} \sum_p \frac{\chi(p)}{p^m} \qquad (2–3) \\ &= -\sum_{\substack{\chi \bmod q \\ \chi \ne \chi_0}} \overline{\chi}(a) \sum_{m \ge 2} \frac{1}{m} \sum_p \frac{\chi(p)}{p^m} + B(q), \end{aligned}$$

where $B(q)$, defined as

$$B(q) := -\sum_{m \ge 2} \frac{1}{m} \sum_{(p,q)=1} \frac{1}{p^m},$$

represents the contribution of the principal character $\chi_0 \bmod q$ and is equal to

$$\begin{aligned} B(q) &= \sum_{(p,q)=1} \left(\log\left(1 - \frac{1}{p}\right) + \frac{1}{p}\right) \\ &= B - \sum_{p \mid q} \left(\log\left(1 - \frac{1}{p}\right) + \frac{1}{p}\right), \end{aligned}$$

where B is defined in (2–2). Recalling from [Languasco and Zaccagnini 09, Section 2] that

$$\begin{aligned} &\varphi(q) \log C(q,a) \qquad (2–4) \\ &\quad = -\gamma + \log\frac{q}{\varphi(q)} - \sum_{\substack{\chi \bmod q \\ \chi \ne \chi_0}} \overline{\chi}(a) \sum_{m \ge 1} \frac{1}{m} \sum_p \frac{\chi(p)}{p^m}, \end{aligned}$$

and comparing the right-hand sides of (2–1), (2–3), and (2–4), it is clear that it is much easier to compute $M(q,a)$ than both $C(q,a)$ and $B(q,a)$, since in (2–1) no prime powers are involved.

Moreover, by (1–3), we can obtain $B(q,a)$ using $M(q,a)$ and $C(q,a)$.

Since in [Languasco and Zaccagnini 09] we already computed several values of $C(q,a)$, it is now sufficient to compute $M(q,a)$ for the corresponding pairs q, a.

To accelerate the convergence of the inner sums in (2–1), (2–3), and (2–4), we will consider, as we did in

[Languasco and Zaccagnini 09], the "tail" of a suitable Euler product. Letting A be a fixed positive integer, we denote the tail of the Euler product of a Dirichlet L-function by

$$L_{Aq}(\chi, s) = \prod_{p>Aq} \left(1 - \frac{\chi(p)}{p^s}\right)^{-1},$$

where $\chi \neq \chi_0 \bmod q$ and $\Re(s) \geq 1$.

For the reader's convenience we give a proof of the following formula:

$$\sum_{p>Aq} \frac{\chi(p)}{p^m} = \sum_{k\geq 1} \frac{\mu(k)}{k} \log(L_{Aq}(\chi^k, km)), \tag{2–5}$$

where $\chi \neq \chi_0 \bmod q$, for every integer $m \geq 1$. We use Möbius inversion with a little care, since the series for $L_{Aq}(\chi, 1)$ is not absolutely convergent. The Taylor expansion for $\log(1-x)$ implies that

$$\begin{aligned}
&\sum_{k\geq 2} \frac{\mu(k)}{k} \log(L_{Aq}(\chi^k, km)) \\
&\quad = \sum_{p>Aq} \sum_{k\geq 2} \sum_{n\geq 1} \frac{\mu(k)}{nkp^{nkm}} \chi^{nk}(p) \\
&\quad = \sum_{p>Aq} \sum_{\ell\geq 2} \frac{\chi^\ell(p)}{\ell p^{\ell m}} \sum_{\substack{k\geq 2 \\ k\mid\ell}} \mu(k) \\
&\quad = -\sum_{p>Aq} \sum_{\ell\geq 2} \frac{\chi^\ell(p)}{\ell p^{\ell m}} \\
&\quad = \sum_{p>Aq} \frac{\chi(p)}{p^m} - \log L_{Aq}(\chi, m),
\end{aligned}$$

since $\sum_{k\mid\ell} \mu(k) = 0$ for $\ell \geq 2$, and this proves (2–5) for every $m \geq 1$.

Now inserting (2–5), with $m = 1$, in (2–1), we have

$$\begin{aligned}
&\varphi(q)M(q,a) \qquad\qquad\qquad\qquad\qquad\qquad (2–6)\\
&\quad = \gamma + B - \sum_{p\mid q} \frac{1}{p} + \sum_{\substack{\chi \bmod q \\ \chi\neq\chi_0}} \overline{\chi}(a) \sum_{p\leq Aq} \frac{\chi(p)}{p} \\
&\qquad + \sum_{\substack{\chi \bmod q \\ \chi\neq\chi_0}} \overline{\chi}(a) \sum_{k\geq 1} \frac{\mu(k)}{k} \log(L_{Aq}(\chi^k, k)) \\
&\quad = \varphi(q) \sum_{\substack{p\leq Aq \\ p\equiv a \bmod q}} \frac{1}{p} + M(q) \\
&\qquad + \sum_{\substack{\chi \bmod q \\ \chi\neq\chi_0}} \overline{\chi}(a) \sum_{k\geq 1} \frac{\mu(k)}{k} \log(L_{Aq}(\chi^k, k)),
\end{aligned}$$

where

$$M(q) := \gamma + B - \sum_{p\mid q} \frac{1}{p} - \sum_{\substack{p\leq Aq \\ (p,q)=1}} \frac{1}{p}.$$

For $A \geq 1$, it is clear that the two sums on the right-hand side of the previous equation collapse to $\sum_{p\leq Aq} 1/p$, but in (3–1) we will explicitly need the value of the summation over $p \mid q$, and hence, to avoid double computations, we will use the definition of $M(q)$ as previously stated.

For $C(q,a)$ the analogue of (2–6) is [Languasco and Zaccagnini 09, equation (5)], while for $B(q,a)$ it can be obtained through a similar argument.

Notice that the Riemann zeta function is never computed at $s = 1$ in (2–6), since for $k = 1$ we have $\chi^k = \chi = \chi_0$. To compute the summation over χ in (2–6) we follow the approach of [Languasco and Zaccagnini 09, Section 2].

This means that in order to evaluate (2–6) using a computer program, we have to truncate the sum over k and to estimate the error we are introducing. Let $K > 1$ be an integer. We get

$$\begin{aligned}
&\varphi(q)M(q,a) \\
&\quad = \varphi(q) \sum_{\substack{p\leq Aq \\ p\equiv a \bmod q}} \frac{1}{p} + M(q) \\
&\qquad + \sum_{\substack{\chi \bmod q \\ \chi\neq\chi_0}} \overline{\chi}(a) \sum_{1\leq k\leq K} \frac{\mu(k)}{k} \log(L_{Aq}(\chi^k, k)) \\
&\qquad + \sum_{\substack{\chi \bmod q \\ \chi\neq\chi_0}} \overline{\chi}(a) \sum_{k>K} \frac{\mu(k)}{k} \log(L_{Aq}(\chi^k, k)) \\
&\quad = \widetilde{M}(q,a,A,K) + E_1(q,a,A,K),
\end{aligned}$$

say. We remark that B, defined as in (2–2), can be easily computed up to 1000 correct digits in a few seconds by adapting (2–3) to the case in which the sum on the left-hand side runs over the complete set of primes. We recall that in [Moree 00], see also the appendix by Niklasch, B and many other number-theoretic constants are computed with a nice precision; see also [Gourdon and Sebah 01]. Using the lemma in [Languasco and Zaccagnini 09] and the trivial bound for χ, it is easy to see that

$$|E_1(q,a,A,K)| \leq \frac{2(Aq)^{1-K}(\varphi(q)-1)}{K^2(Aq-1)}.$$

We take this occasion to correct a typo in the inequality for $E_1(q,a,A,K)$ in [Languasco and Zaccagnini 09, p. 319]: the factor $2K$ in the denominator should read K^2.

In order to ensure that $\widetilde{M}(q,a,A,K)$ is a good approximation of $M(q,a)$, it is sufficient that Aq and K be sufficiently large. Setting $Aq = 9600$ and $K = 26$ yields the desired 100 correct decimal digits.

Now we have to consider the error we are introducing during the evaluation of the Dirichlet L-functions that appear in $\widetilde{M}(q,a,A,K)$. This can be done exactly as in [Languasco and Zaccagnini 09, Section 3], with km there replaced by k.

Let T be an even integer and N a multiple of q. For $\chi \neq \chi_0 \bmod q$ and $k \geq 1$, we use the Euler–Maclaurin formula in the following form:

$$\begin{aligned} &L_{T,N}(\chi^k, k) \qquad\qquad (2\text{–}7)\\ &\quad = \sum_{r<N} \frac{\chi^k(r)}{r^k}\\ &\qquad - \frac{1}{N^k}\sum_{j=1}^{T} \frac{(-1)^{j-1}B_j(\chi^k)}{j!}\frac{k(k+1)\cdots(k+j-2)}{N^{j-1}}, \end{aligned}$$

where $B_n(\chi)$ denotes the χ-Bernoulli number, which is defined by means of the nth Bernoulli polynomial $B_n(x)$ (see [Cohen 07, Definition 9.1.1]), as follows:

$$B_n(\chi) = f^{n-1}\sum_{a=0}^{f-1}\chi(a)B_n\left(\frac{a}{f}\right),$$

in which f is the conductor of χ.

Hence the error term in evaluating the tail of the Dirichlet L-functions $L_{Aq}(\chi^k, k)$ is

$$\begin{aligned} &|E_2(q,a,K,N,T)|\\ &\quad \leq \frac{(\varphi(q)-1)q^T B_T}{U(q,K,N,T)} \sum_{1\leq k\leq K} \frac{1}{k}\frac{k\cdots(k+T-2)}{T!}N^{1-k-T}\\ &\quad = \frac{(\varphi(q)-1)q^T B_T}{U(q,K,N,T)T!}\\ &\qquad \times \sum_{1\leq k\leq K}(k+1)\cdots(k+T-2)N^{1-k-T}\\ &\quad \leq \frac{(\varphi(q)-1)(K+T-2)^{T-2}q^T B_T}{U(q,K,N,T)N^{T-1}T!}\sum_{1\leq k\leq K}N^{-k}\\ &\quad \leq \frac{2(\varphi(q)-1)(K+T-2)^{T-2}q^T B_T}{(N-1)U(q,K,N,T)N^{T-1}T!}, \end{aligned}$$

where B_T is the Tth Bernoulli number, which is the Tth coefficient of the power series expansion of the function $x/(e^x-1)$, and

$$U(q,K,N,T) := \min_{\substack{\chi \bmod q\\ \chi\neq\chi_0}} \min_{1\leq k\leq K} |L_{T,N}(\chi^k, k)|.$$

Collecting the previous estimates, we have that

$$\left| M(q,a) - \frac{\widetilde{M}(q,a,A,K)}{\varphi(q)} \right| \leq \frac{|E(q,a,A,K,N,T)|}{\varphi(q)},$$

where $E(q,a,A,K,N,T)$ denotes

$$E_1(q,a,A,K) + E_2(q,a,K,N,T).$$

Some experimentation for $q \in \{3,\ldots,100\}$ suggested to us that we use different ranges for N and T to reach a precision of at least 100 decimal digits in a reasonable amount of time. Using $Aq = 9600$, $K = 26$ and recalling that $q \mid N$ and T is even, our choice is $N = (\lfloor 8400/q \rfloor + 1)q$ and $T = 58$ if $q \in \{3,\ldots,10\}$, while for $q \in \{90,\ldots,100\}$ we have to use $N = (\lfloor 27720/q \rfloor + 1)q$ and $T = 88$. Intermediate ranges are used for the remaining integers q.

The programs we used to compute the Dirichlet characters modulo q and the values of $M(q,a)$ for $q \in \{3,\ldots,100\}$, $1 \leq a \leq q$, $(q,a) = 1$, were written using the GP scripting language of Pari/GP.[1] The C program was obtained from the analogous GP program using the `gp2c` tool. The actual computations were performed using a double quad-core Linux PC for a total amount of computing time of about four hours and four minutes. The complete set of results is available online (http://www.math.unipd.it/~languasc/Mertens-comput.html), together with the source program in GP and the results of the verifications of the identities (3–1) and (3–2), which are described in the following section.

Moreover, at the same web address, you will also find the values of $B(q,a)$ computed via (1–3) using the previous results on $M(q,a)$ and those for $C(q,a)$ in [Languasco and Zaccagnini 09]. The use of (1–3) implies some sort of "error propagation." To avoid this phenomenon we recomputed some values of $C(q,a)$. A complete report of this recomputation step can be found at the web address previously mentioned.

Moreover, to be safer, we also directly computed $B(q,a)$ using (2–3) for $q \in \{3,\ldots,100\}$, $1 \leq a \leq q$, and $(q,a) = 1$. The computation time was about three days, six and one-fourth hours. By comparing the values of $B(q,a)$ obtained using these two methods, we can say with confidence that the values of $B(q,a)$ we computed are correct up to 100 decimal digits.

Finally, we also wrote a program to compute $B(q,a)$, $C(q,a)$, and $M(q,a)$ with at least 20 correct decimal digits. Comparing with [Languasco and Zaccagnini 09], the

[1] Available online (http://pari.math.u-bordeaux.fr/).

main parameters can be chosen now to be much smaller, and so we were able to compute all these constants for every $3 \le q \le 300$, $1 \le a \le q$, $(q,a) = 1$. In particular, the required time on a double quad-core Linux PC for the range $q \in \{3, \dots, 200\}$ was about five hours and five minutes, while for the range $q \in \{201, \dots, 300\}$, it was about eighteen hours. In this case we directly computed $B(q,a)$, $C(q,a)$, and $M(q,a)$ and we used (1–3) as a consistency check.

All of these results can be downloaded at the web address previously mentioned.

3. VERIFICATION OF CONSISTENCY

The set of constants $M(q,a)$ satisfies many identities, and we checked our results verifying that these identities hold within a very small error. The basic identities that we exploited are two: the first is

$$\sum_{\substack{a \bmod q \\ (q,a)=1}} M(q,a) = \gamma + B - \sum_{p \mid q} \frac{1}{p}. \tag{3–1}$$

This can be verified by a direct computation, taking into account the fact that primes dividing q do not occur in any sum of the type

$$\sum_{\substack{p \le x \\ p \equiv a \bmod q}} \frac{1}{p}.$$

The other identity is valid whenever we take two moduli q_1 and q_2 with $q_1 \mid q_2$ and $(a, q_1) = 1$. In this case we have

$$M(q_1, a) = \sum_{\substack{j=0 \\ (a+jq_1, q_2)=1}}^{n-1} M(q_2, a + jq_1) + \sum_{\substack{p \mid q_2 \\ p \equiv a \bmod q_1}} \frac{1}{p}, \tag{3–2}$$

where $n = q_2/q_1$.

Equation (3–2) holds also for $B(q,a)$ with the only remark that in the final summation, the summand $1/p$ should be replaced by $\log(1 - 1/p) + 1/p$. Concerning (3–1), this holds for $B(q,a)$ too if we replace $\gamma - \sum_{p \mid q} 1/p$ with $-\sum_{p \mid q} (\log(1 - 1/p) + 1/p)$.

The proof of (3–2) depends on the fact that the residue class $a \bmod q_1$ is the union of the classes $a + jq_1 \bmod q_2$, for $j \in \{0, \dots, n-1\}$. If q_1 and q_2 have the same set of prime factors, the condition $(a + jq_1, q_2) = 1$ is automatically satisfied, since $(a, q_1) = 1$ by our hypothesis.

On the other hand, if q_2 has a prime factor p that q_1 lacks, then there are values of j such that $p \mid (a + jq_1, q_2)$ and the corresponding value of $M(q_2, a + jq_1)$ on the right-hand side of (3–2) would be undefined. The sum at the far right takes into account these primes.

The validity of (3–1) was checked immediately at the end of the computation of the constants $M(q,a)$, for a fixed q and for every $1 \le a \le q$ with $(q,a) = 1$, by the same program that computed them. These results were collected in a file, and a different program checked that (3–2) holds within a very small error by building every possible relation of that kind for every $q_2 \in \{3, \dots, 100\}$ and $q_1 \mid q_2$ with $1 < q_1 < q_2$. As in [Languasco and Zaccagnini 09], the total number of identities checked was

$$\sum_{q=3}^{100} \sum_{\substack{d \mid q \\ 1<d<q}} \varphi(d) = \sum_{q=3}^{100} (q - 1 - \varphi(q)) = 1907,$$

but there are dependencies among them, which we did not bother to eliminate, since the total time required for this part of the computation is absolutely negligible. Again as in [Languasco and Zaccagnini 09], the number of independent identities is

$$\sum_{q=3}^{100} \sum_{\substack{p \mid q \\ p<q}} \varphi\left(\frac{q}{p}\right) = \sum_{n=2}^{100} \pi\left(\frac{100}{n}\right) \varphi(n) = 1383,$$

where p denotes a prime in the sum on the left. Please note that in [Languasco and Zaccagnini 09, p. 323], we erroneously wrote that the previous sum is equal to 1408, which is in fact its value starting from $n = 1$.

Similar checks were done also for the 20-digit case. Working for every $q \le 300$, we have 12,343 independent relations over a total number of 17,453 such relations. In this case, too, we obtained the desired precision (at least 20 decimal digits).

4. APPENDIX (BY K. K. NORTON): PROOF OF CONJECTURE (1–4)

The proof is a direct consequence of the following lemma by Karl K. Norton.

Lemma 4.1. (Lemma 6.3 of [Norton 76]). *Let $q \ge 2$ be an integer and let L be a nonempty set of integers such that for each $a \in L$, we have $1 \le a < q$ and $(q,a) = 1$.*

Write $|L| = \lambda$ for the cardinality of L, and let $E = \bigcup_{a \in L} \{p \text{ prime} : p \equiv a \bmod q\}$. Then, for $x \ge 2$, we have

$$\sum_{\substack{p \le x \\ p \in E}} \frac{1}{p} = \lambda \frac{\log\log x}{\varphi(q)} + \sum_{\substack{p \le x \\ p \in L}} \frac{1}{p} + \mathcal{O}\left(\lambda \frac{\log q}{\varphi(q)}\right), \tag{4–1}$$

where the implicit constant is absolute. Also,

$$\sum_{\substack{p\le x\\ p\in L}} \frac{1}{p} \le \log\log(3\lambda) + \mathcal{O}(1),$$

where the implicit constant is absolute.

Taking just one fixed arithmetic progression $p \equiv a \bmod q$, with $1 \le a < q$ and $(q,a) = 1$, (this means $L = \{a\}$) equation (4–1) implies, for $x \ge 2$, that

$$\sum_{\substack{p\le x\\ p\equiv a \bmod q}} \frac{1}{p} = \frac{\log\log x}{\varphi(q)} + f(a) + \mathcal{O}\left(\frac{\log q}{\varphi(q)}\right), \qquad (4\text{–}2)$$

where $f(a) = 1/a$ if a is a prime number and 0 otherwise, and the implicit constant is absolute. Combining this with (1–1) we get immediately that

$$M(q,a) = \begin{cases} 1/a + \mathcal{O}\left(\frac{\log q}{\varphi(q)}\right) & \text{if } a \text{ is a prime number,}\\ & \quad 1 \le a < q,\ (q,a) = 1,\\ \mathcal{O}\left(\frac{\log q}{\varphi(q)}\right) & \text{if } a \text{ is not a prime number,}\\ & \quad 1 \le a < q,\ (q,a) = 1,\end{cases}$$

and hence (1–4) holds.

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