Computation of large values of $\pi(x)$

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[summary by Philippe Dumas and François Morain]

Every textbook about number theory explains the sieve of Eratosthenes [3], which is one of the oldest known algorithms. This algorithm enables us to compute the prime numbers less than a fixed number x. It consists in successively striking out the multiples of the already known prime numbers, the first one being 2. The cost of the algorithm is $O(x^{1+\varepsilon})$ for all $\varepsilon > 0$. Pritchard has given a lot of theoretical algorithms that perform in sublinear time (see [8] for new results and a bibliography on this topic). From a practical point of view, many tricks can be used to find all primes less than 10^{12} in a fast way, as explained for example in [1].

Clearly the enumeration of all the primes less than x cannot have a lower cost than $\pi(x)$. Besides the computation of $\pi(x)$, the number of primes less or equal to x, does not need to find all the primes less than x. This fact is set up by the formula of Legendre, which uses the prime numbers less or equal to $\sqrt{x}$. Next, the works of Meissel and Lehmer provides more subtle formulæ, which reduce the amount of computation. As an example Meissel computed the value of $\pi(10^8)$. Nevertheless, these methods all have a cost of $O(x^{1+\varepsilon})$. Lagarias, Miller, and Odlyzko gave a method which for the first time had a complexity $O(x^\alpha)$ with $\alpha < 1$. More precisely the time complexity is $O(x^{2/3+\varepsilon})$ and the space complexity is $O(x^{1/3+\varepsilon})$. This permits them to compute the value of $\pi(10^{16})$. Deléglise and Rivat [2] lessen the time complexity by a logarithmic factor using a slight modification of the previous method, hence they obtained the value of $\pi(10^{18})$.

All these methods use the idea of sieve, but Lagarias and Odlyzko [5] proposed an entirely different way to compute $\pi(x)$. The method is based on an analytic formula, and its expected cost is $O(x^{1/2+\varepsilon})$. It has never been implemented.

1. Sieve function

Let us assume that we use the sieve of Eratosthenes. We write all the integers between 1 and x, and we strike out successively the multiples of $p_1 = 2$, $p_2 = 3$, and so on. We stop when we have used the a-th prime number p_a. The number of integers which remain is $\phi(x,a)$. The function $\phi(x,a)$ is the partial sieve function. As a convention, we set $\phi(x,0) = \lfloor x \rfloor$. A mere combinatorial argument gives the following recursion rule,

$$\phi(x,a) = \phi(x,a-1) - \phi(x/p_a, a-1).$$

A raw application of this rule gives the formula

$$\phi(x,a) = \sum_{\substack{m \le x \\ P(m) \le p_a}} \mu(m) \lfloor x/m \rfloor,$$

where $\mu(m)$ is the Möbius function and $P(m)$ is the largest prime factor of m.

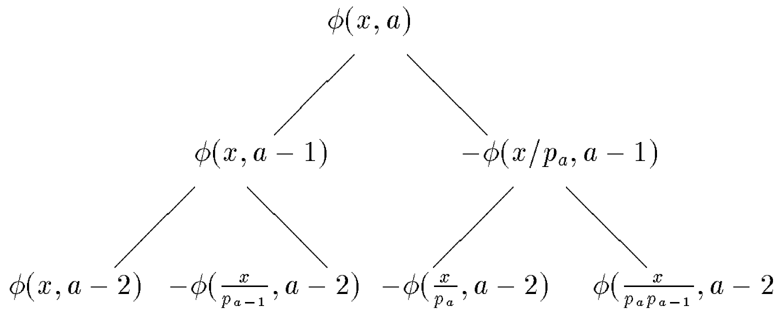

FIGURE 1. A computation tree for $\phi(x,a)$. The sum of the leaves is $\phi(x,a)$.

In the sequel, an important point will be a clever refinement in the use of the recursion rule. Indeed the last formula contains too many terms. The recursion rule may be viewed as an expansion rule, which provides a computation tree for $\phi(x,a)$ (see Fig. 1). The problem is to give a stopping criterion in order to avoid an excessive growth of the number of leaves.

The partial sieve function $\phi(x,a)$ is used in the following manner. Let us denote by $P_k(x,a)$ the number of integers less or equal to x with exactly k equal or distinct prime factors, those prime factors being all greater than p_a. With the equality $P_0(x,a)=1$, we have immediately

$$\phi(x,a) = P_0(x,a) + P_1(x,a) + P_2(x,a) + P_3(x,a) + \cdots .$$

But it is manifest that

$$P_1(x,a) = \pi(x) - a,$$

hence the following basic formula

$$\pi(x) = \phi(x,a) - 1 + a + P_2(x,a) + P_3(x,a) + \cdots . \tag{1}$$

With $a=\pi(\sqrt{x})$, the quantities $P_k(x,a)$ are zero for $k>2$ because any composite number with three prime factors larger than $\sqrt{x}$ is larger than x. Hence, we obtain Legendre's formula [9]

$$\pi(x) = \phi(x,a) + a - 1, \qquad a = \pi(\sqrt{x}).$$

An expanded form of this formula is

$$\pi(x) = \pi(\sqrt{x}) - 1 + \sum_H (-1)^{\#H} \lfloor x/p_H \rfloor,$$

where H runs through the subsets of $\{1,2,\ldots,\pi(\sqrt{x})\}$ and $p_H = \prod_{h\in H} p_h$. The computation of $\pi(x)$ based on this formula has cost $O(x)$.

2. Meissel and Lehmer

Meissel chose the value $a=\pi(x^{1/3})$ in the basic formula (1), hence the formula reduces to

$$\pi(x) = \phi(x,a) + a - 1 + P_2(x,a), \qquad a = \pi(x^{1/3}). \tag{2}$$

The most time consuming part of the formula is the term $\phi(x,a)$ and Lehmer proposed the following truncation rule for the computation tree of Figure 1:

> Do not split a node labelled $\pm\phi(x/n,b)$ if either of the following holds:
> (i) $x/n < p_b$,
> (ii) $b=5$.

Lehmer used $a = \pi(x^{1/4})$ and the tree has leaves labelled by $\pm\phi(x/n, b)$ for n a product of four prime numbers between $p_6 = 13$ and p_a; this leads to a number of leaves essentially of order x. For a detailed description of the implementation, see the original article of Lehmer [6] or the problem [7, Problème 5].

3. Lagarias, Miller, and Odlyzko

In [4], Lagarias, Miller, and Odlyzko use a sharper truncation rule, namely

Do not split a node labelled $\pm\phi(x/n, b)$ if either of the following holds:
(i) $b = 0$ and $n \leq x^{1/3}$,
(ii) $n > x^{1/3}$.

They use $a = \pi(x^{1/3})$ and for this value the number of leaves of the computation tree is no more than $O(x^{2/3})$. The leaves associated with the case (i) are the *ordinary leaves*, and the leaves associated with the case (ii) are the *special leaves*.

According to (2) there are two terms to compute: $\phi(x, a)$ and $P_2(x, a)$. The computation has four steps; first a preparatory step; next the computation of $P_2(x, a)$; then the computation of the contribution of the ordinary leaves; finally the computation of the special leaves. The sum which correspond to $\phi(x, a)$ is the sum of these last two quantities.

Preparatory step. Using an ordinary Eratosthenes sieve, one finds all the primes $p_1, p_2, \ldots, p_a$ below $x^{1/3}$. During the sieving, several quantities are also computed and stored for a later use. When sieving with p_i, the values of the Möbius function $\mu(n)$ for $n \leq x^{1/3}$ can be updated. The values of the function f which gives the least prime factor of an integer n in the interval is computed too. Having sieved with the i-th prime, the value of $\phi(x^{1/3}, i)$ is known and stored.

Finally, the value $\pi(x^{1/4})$ is computed. All this has a cost $O(x^{1/3+\varepsilon})$ arithmetic operations and space cost $O(x^{1/3})$.

Computation of $P_2(x, a)$. The quantity $P_2(x, a)$ is computed according to the formula

$$P_2(x, a) = \binom{a}{2} - \binom{a'}{2} + \sum_{x^{1/3} < p \leq x^{1/2}} \pi(x/p), \qquad a = \pi(x^{1/3}), \quad a' = \pi(x^{1/2}).$$

The computation of the Meissel sum

$$\sum_{x^{1/3} < p \leq x^{1/2}} \pi(x/p)$$

needs to count the prime numbers in the interval $[x^{1/3}, x^{2/3}]$. This interval is sieved slice by slice, where the slices are intervals of width $x^{1/3}$. The computation uses for each slice an auxiliary sieve, in order to determine the prime numbers p such that x/p falls in the current slice. The value of π is updated during the handling of the slice. The value of $\pi(x^{1/2})$ is stored when the suitable slice is processed.

Estimating the contribution of ordinary leaves. During the preceding step the sum associated to the ordinary leaves

$$\sum_{1 \leq n \leq x^{1/3}} \mu(n) \lfloor x/n \rfloor$$

is also computed.

Estimating the contribution of special leaves. This is the most intricate part of the method. We have to evaluate

$$S = \sum_{(n,b)} \mu(n)\phi(x/n, b)$$

for all special leaves (n, b), i.e., $n = p_{a_1} \cdots p_{a_r}$ with $a \geq a_1 > a_2 > \cdots > a_r = b + 1$ and $n \geq x^{1/3} \geq n/p_{b+1}$.

We will evaluate this sum by sieving the interval $[x^{1/3}, x^{2/3}]$ by subintervals of length $x^{1/3}$. Let $N = \lfloor x^{1/3} \rfloor$. Suppose the number x/n is in the k-th subinterval $[(k-1)N + 1, kN]$. Then (n, b) is a special leaf if and only if $n = n^* p_{b+1}$, $f(n^*) > p_{b+1}$ and

$$\frac{x}{(kN+1)p_{b+1}} < n^* \leq \frac{x}{((k-1)N+1)p_{b+1}}.$$

In other words, n^* belongs to an interval $[L, M]$ and the contribution of $(x/n, b)$ to the sum S is non-zero if and only if $\mu(n^*) \neq 0$. This shows the process: we loop through those numbers m in $[L, M]$ such that $f(m) > p_{b+1}$ and for which $\mu(m) \neq 0$. This is easy using the tables precomputed in phase 1. In order to complete the evaluation, one must set up the computations in a clever way, described in the original paper (see also [2]). This crude description yields an algorithm with time $O(x^{2/3})$ which can be lowered to $O(x^{2/3}/\log x)$ using a trick due to Miller and described in the paper.

At the end, the values of a, $P_2(x, a)$ and $\phi(x, a)$ are combined and $\pi(x)$ is obtained. The total time for computing $\pi(x)$ is thus $O(x^{2/3}/\log x)$ operations and $O(x^{1/3}\log^2 x \log\log x)$ space.

4. Deléglise and Rivat

In [2], the authors describe a variant of the above approach that uses $O(x^{2/3}/\log^2 x)$ operations and $O(x^{1/3}\log^3 x \log\log x)$ space. They have computed all values of $\pi(x)$ for $x \geq 10^{15}$ up to 10^{18} for which $\pi(10^{18}) = 24739954287740860$.

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