THE COMBINATORIAL METHOD TO COMPUTE THE SUM OF THE POWERS OF PRIMES

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ABSTRACT. We will generalize the combinatorial algorithms for computing $\pi(x)$ to compute sums $F(x) = \sum_{p \leq x} p^k$ for $k \in \mathbb{Z}_{\geq 0}$. The detailed exposition of algorithms is included along with implementation details.

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1. INTRODUCTION

The history of the calculation of $\pi(x)$ without enumerating all the primes up to $x$ dates back to Legendre. His method was combinatorial at heart and was based on the Inclusion-Exclusion Principle, requiring primes up to $\sqrt{x}$. The next step was done by Meissel in 1870, and later by Lehmer \[1\] in 1959, who streamlined the
Meissel’s algorithm into what would be later called Meissel-Lehmer algorithm. Next improvements came from Lagarias, Miller, Odlyzko [2] in 1985, and from Deleglise, Rivat [1] in 1996. Later improvements were mainly concerned with implementation improvements and are of no interest to us here. All these algorithm are “combinatorial”, as opposed to “analytical” methods that were inspired by the works of Lagarias, Odlyzko [3]. Our goal is to generalize the “combinatorial” method to calculate not just \( \pi(x) = \sum_{p \leq x} p^0 \), but the more general sum \( F_k(x) = \sum_{p \leq x} p^k \) for \( k \) non-negative integer.

We will give a self-contained exposition of the “combinatorial” algorithm for calculating \( F_k(x) \) and provide some values of \( F_k(x) \) for \( k = 2, 3, 4 \).

2. GENERAL DESCRIPTION

We shall start with describing the combinatorial method, closely following [4]. Let

\[
F(x) = \sum_{p \leq x} f(p),
\]

where \( f \) is completely multiplicative. We write

\[
m_a = \prod_{i \leq a} p_i
\]

for the product of the first \( a \) primes.

By \( \phi(x, a) \) we denote the sum of \( f(n) \) over the numbers \( n \leq x \) divisible by none of the first \( a \) primes:

\[
\phi(x, a) = \sum_{n \leq x \atop (n, m_a) = 1} f(n);
\]

and by \( P_k(x, a) \) we denote the sum of \( f(n) \) over \( n \leq x \) such that \( n \) is a product of \( k \) primes each greater than \( p_a \):

\[
P_k(x, a) = \sum_{p_a < q_1 \ldots q_k \leq x} f(q_1 \ldots q_k).
\]

Also, by the usual convention, we set \( P_0(x, a) = f(1) = 1 \).

We clearly see that

\[
\phi(x, a) = \sum_{k=1}^{\infty} P_k(x, a).
\]

Further, for \( k \) such that \( x < p_{a+1}^k \) we have \( P_k(x, a) = 0 \), and upon writing \( r \) for the smallest such \( k \), we may rewrite this sum as \( \phi(x, a) = \sum_{k=0}^{r-1} P_k(x, a) \).

We can also go in the “opposite” direction: fixing \( r \), i.e. limiting the number of \( P_k \), we will acquire the bounds on \( a \):

\[
a \in \left[ \pi \left( x^{\frac{1}{r+1}} \right), \pi \left( x^{\frac{1}{r-1}} \right) \right].
\]

We fix a parameter \( Y \) such as

\[
x^{\frac{1}{r}} \leq Y < x^{\frac{1}{r-1}},
\]

and set \( a = \pi(Y) \). We will return to the choice of \( Y \) later, when we will use it to balance different parts of computation to achieve optimal performance.
After we expand $P_1$:

$$P_1(x, a) = \sum_{p_a < p \leq x} f(p) = F(x) - F(p_a),$$

we may rewrite the sum as

$$F(x) = \phi(x, a) + F(p_a) - 1 - \sum_{k=2}^{r-1} P_k(x, a),$$

thus the computation of $F$ is reduced to the computation of $P_k$ and $\phi$.

We shall start with the computation of $\phi$. We define $Q(x, k) = \sum_{ik \leq x} f(ik)$ and we shall prove that $\phi(x, a) = \sum_{d|m_a} \mu(d)Q(x, d)$.

$$\sum_{d|m_a} \mu(d)Q(x, d) = \sum_{d|m_a} \mu(d) \sum_{d|m} f(m) = \sum_{m \leq x} f(m) \sum_{d|(m, m_a)} \mu(d)$$

$$= \sum_{m \leq x} f(m) = \phi(x, a).$$

We now split all the divisors $d$ of $m_a$ in two groups.

The contribution of $d$ such that $p_a \nmid d$ is

$$\sum_{d|m_a, p_a \nmid d} \mu(d)Q(x, d) = \sum_{d|m_{a-1}} \mu(d)Q(x, d) = \phi(x, a - 1),$$

and for the rest

$$\sum_{p_a|d} \mu(d)Q(x, d) = \sum_{d|m_{a-1}} \mu(p_a d)Q(x, p_a d) = -\sum_{d|m_{a-1}} \mu(d) \sum_{d|m, m \leq x} f(m)$$

$$= -f(p_a) \sum_{d|m_{a-1}} \mu(d) \sum_{d|m, m \leq x/p_a} f(m)$$

$$= -f(p_a)\phi\left(\frac{x}{p_a}, a - 1\right),$$

giving us

$$\phi(x, a) = \phi(x, a - 1) - f(p_a)\phi\left(\frac{x}{p_a}, a - 1\right).$$

As $\phi(x, 0) = \sum_{n \leq x} f(n)$ we see that this recursive formulation may be represented as a binary tree of the height $a$. 

Next we shall expand $P_2$ and $P_3$:

\[
P_2(x, a) = \sum_{p_a < p_i, p_j \leq \sqrt{x}} f(p_i p_j) = \sum_{a < i \leq \pi(\sqrt{x})} f(p_i) \sum_{i \leq j \leq \pi(\sqrt{x})} f(p_j)
\]

\[
= \sum_{a < i \leq \pi(\sqrt{x})} f(p_i) \left[ F\left(\frac{x}{p_i}\right) - F(p_i - 1) \right].
\]

\[
P_3(x, a) = \sum_{p_a < p_i, p_j, p_k \leq \sqrt{x}} f(p_i p_j p_k)
\]

\[
= \sum_{a < i \leq \pi(\sqrt{x})} f(p_i) \sum_{i \leq j \leq \pi(\sqrt{x})} f(p_j) \sum_{j \leq k \leq \pi(\sqrt{x})} f(p_k)
\]

\[
= \sum_{a < i \leq \pi(\sqrt{x})} f(p_i) \sum_{i \leq j \leq \pi(\sqrt{x})} f(p_j) \left[ F\left(\frac{x}{p_i p_j}\right) - F(p_j - 1) \right].
\]

We see that the sum for $P_3$ is way more complicated than $P_2$, this is the price we pay to lower $a$ from $3\sqrt{x}$ to $4\sqrt{x}$. Thankfully, as we will see later, in the case of $r = 3$ we can optimize the computation of $\phi(x, a)$ in such a way that we will need the “recursive” procedure above only for $\phi(x, 4\sqrt{x})$, thus making the addition of $P_3$ unneeded.

Hence, from now on, we fix $r = 3$, and we consider $Y$ such that $\sqrt{x} \leq Y < \sqrt{x}$, to be a parameter, setting $a = \pi(Y)$. We shall now consider the computation of $\phi(x, a)$ and $P_2$ in greater detail.

3. Computing $P_2(x, a)$

We recall the formula for calculating $P_2$:

\[
P_2(x, a) = \sum_{p_a < p_i \leq \sqrt{x}} \left[ F\left(\frac{x}{p_i}\right) - F(p_i - 1) \right]
\]

\[
= \sum_{p_a < p_i \leq \sqrt{x}} f(p) F\left(\frac{x}{p_i}\right) - \sum_{p_a < p_i \leq \sqrt{x}} f(p) F(p_i - 1).
\]

We write $P_2(x, a) = S_1 - S_2$, where

\[
S_1 = \sum_{a < i \leq \pi(\sqrt{x})} f(p_i) F\left(\frac{x}{p_i}\right)
\]

\[
S_2 = \sum_{a < i \leq \pi(\sqrt{x})} f(p_i) F(p_i - 1)
\]

For calculating $S_2$, we note that we can accumulate $F(p_i - 1)$ as we go through primes in $(p_a, \sqrt{x}]$.

To calculate $S_1$ we need to know the values of $F(\pi/p_i)$ and we have

\[
\sqrt{x} \leq \frac{x}{p_i} \leq \frac{x}{p_a + 1} < \frac{x}{Y}.
\]

We write

\[
L = \left\lfloor \sqrt{x} \right\rfloor, R = \left\lceil \frac{x}{Y} \right\rceil
\]
and proceed by sieving the interval \([L, R]\) in blocks \(I_k = [L + (k - 1)B, L + kB]\) of size \(B\), with the possible exception of the last block which can be shorter. As we have \(\frac{x}{p_i} \in I_k\), it is natural to consider the block

\[ J_k = \left( \frac{x}{L + kB}, \frac{x}{L + (k - 1)B} \right) \cap \left( Y, \sqrt[x]{x} \right), \]

and sieve it completely. In the end we know all the primes \(p_i\) such that \(x^{p_i} \in I_k\). As we have sieved \(I_k\) fully we can calculate \(F(x^{p_i})\) easily, so we just add \(f(p_i)F(x^{p_i})\) to the \(S_1\) accumulator.

We should estimate the maximal length of \(J_k\). Suppose we consider \(I_k = [h - B, h)\), with \(h > \sqrt[x]{x}\). Then

\[ \frac{x}{h - B} - \frac{x}{h} = \frac{xB}{h(h - B)}. \]

If we assume that \(h - B \geq \sqrt[x]{x}\) (that is the usual block for \(S_1\) calculation) then \(h(h - B) \geq x\), and we clearly don’t need more than \(B\) integers.

On the other hand, if \(h - B < \sqrt[x]{x}\), we would have \(J_k\) shortened to \(\left( \frac{x}{h}, \sqrt{x} \right)\) and then

\[ \sqrt{x} - \frac{x}{h} = \frac{h\sqrt{x} - x}{h} \leq \frac{h\sqrt{x} - x}{\sqrt{x}} = h - \sqrt{x} < B, \]

and again, we don’t need more than \(B\) integers.

4. Computing \(\phi(x, a)\)

4.1. Recursion Tree. It is clear that as we go through the recursion

\[ \phi(x, a) = \phi(x, a - 1) - f(p_a)\phi(x/p_a, a - 1), \]

we obtain a binary tree, and ultimately we need to sum the leaf values. The nodes of the tree are of the form

\[ \mu(n)f(n)\phi\left( \frac{x}{n}, b \right), \]

where \(n = p_{i_1} \cdots p_{i_r}, a \geq a_1 > \cdots > a_r > b\),

and we will label them with \((n, b)\).

Now, we need to consider the possibility of the “truncation” of our tree. We will consider the case when \(b\) is “small”, and when \(n\) is “large” (i.e. \(x/n\) is “small”).

The very first truncation rule is quite obvious: for \(z \leq p_k\) we have \(\phi(z, k) = 1\), and thus we have

**The Truncation Rule** \(T_0\) Stop at the node \((n, b)\) if either of the following holds:

1. \(n \geq x/p_b\)
2. \(n < x/p_b\), and \(b = 0\).

We shall write \(\phi_m\) for the \(\phi\) function corresponding to \(f(n) = n^m\). In [4] it was proposed to tabulate the values of \(\phi_0(x, a)\) for small values of \(a\) when computing \(\pi(x)\), and we shall generalize this. Let \(P\) be the product of the first \(K\) primes. Now we shall consider the task of calculating \(\phi_m(x, K)\), having

\[ x = qP + r \text{ with } 0 \leq r < P. \]
Assuming that we have precomputed $\phi_m(n, K)$ for $n \leq P$ we use the Binomial theorem to obtain

$$
\phi_m(x, K) = \sum_{i=0}^{q-1} \sum_{j<P} \sum_{(j,P)=1} (iP + j)^m + \sum_{j<r} \sum_{(j,P)=1} (qP + j)^m
$$

$$
= \sum_{i=0}^{q-1} \sum_{j<P} \sum_{k=0}^{m} \left( \frac{m}{k} \right) i^k P^k j^{m-k} + \sum_{j<r} \sum_{k=0}^{m} \left( \frac{m}{k} \right) q^k P^k j^{m-k}
$$

$$
= \sum_{k=0}^{m} \left( \frac{m}{k} \right) P^k \sum_{i=0}^{q-1} i^k \sum_{j<P} j^{m-k} + \sum_{k=0}^{m} \left( \frac{m}{k} \right) q^k P^k \sum_{j<r} j^{m-k}
$$

$$
= \sum_{k=0}^{m} \left( \frac{m}{k} \right) P^k \phi_{m-k}(P-1, K) \sum_{i=0}^{q-1} i^k + \sum_{k=0}^{m} \left( \frac{m}{k} \right) q^k P^k \phi_{m-k}(r, K)
$$

$$
= \sum_{k=0}^{m} \left( \frac{m}{k} \right) P^k \left( \phi_{m-k}(P-1, K) \sum_{i=0}^{q-1} i^k + \phi_{m-k}(r, K)q^k \right).
$$

We may assume, that we can calculate $\sum_{i=0}^{q-1} i^k$ for a fixed $k$ efficiently, and then we need to store the values of $\phi_0(x, K), \ldots, \phi_m(x, K)$ for $x < P$. Thus we can update our truncation rule:

**The Truncation Rule** $T_1(K)$ Stop at the node $(n, b)$ if either of the following holds:

1. $n \geq \frac{x}{p_b}$
2. $n < \frac{x}{p_b}$, and $b = K$.

We shall briefly note that setting $K = 0$ gives us the initial truncation rule.

Now we will update the truncation rule for “large” $n$, following [2]:

**The Truncation Rule** $T_2(Y, K)$ Stop at the node $(n, b)$ if either of the following holds:

1. $n > Y$
2. $n \leq Y$, and $b = K$.

We will call the leaves of type 1 *special leaves* and of type 2 *ordinary leaves*.

At this point we should prove the correctness of this rule, i.e. that we account for all the nodes, and exactly once. Consider the level of the tree corresponding to $K$, consisting of the nodes $(n, K)$. Since we go through the primes in descending order we clearly have $(P, n) = 1$, namely $n$ is not divisible by the first $K$ primes. On this level we have ordinary nodes $(n, K)$ with $n \leq Y$, and the nodes with $n > Y$, which can be backtracked to the special node.

Therefore we have

$$
\phi(x, a) = \sum_{(n, K) \, \text{ordinary}} \mu(n)f(n)\phi\left(\frac{x}{n}, K\right) + \sum_{(n, b) \, \text{special}} \mu(n)f(n)\phi\left(\frac{x}{n}, b\right).
$$

We note that the contribution of the ordinary leaves can be computed immediately, as it is the sum over squarefree $n \leq Y$ such that $(n, P) = 1$, and the terms can be computed efficiently. Thus the special leaves make up the core essence of the calculation.
4.2. Special Leaves. For the special leaf \((n, b)\) we note that its parent couldn’t be \((n, b + 1)\) as we would stop earlier. Hence it was \((n^*, b + 1)\), with \(n = n^*p_{b+1}\), and we have \(n^* \leq Y < n^*p_{b+1}\), \(l_p(n) = p_{b+1}\) where we write \(l_p(n)\) for the smallest prime factor of \(n\); as we go through the primes in descending order we must have \(l_p(n^*) > p_{b+1}\). Thus the multiplier for the node \((n, b)\) is

\[
\mu(n)f(n) = \mu(n^*)\mu(p_{b+1})f(n^*)f(p_{b+1}) = -\mu(n^*)f(n^*)f(p_{b+1}).
\]

We might go through the primes \(p_k\) with \(k \in [1, a]\) and enumerate squarefree \(n^* \in [Y/p_k, Y]\), with \(l_p(n^*) > p_k\), calculating \(\phi\) recursively.

We shall now describe the procedure to compute the contribution of special leaves without recursion. We note that we can actually compute \(\phi(x, a)\) iteratively in blocks. Consider the block \(I = [l, h)\) of length \(B = h - l\) and suppose that we know \(\phi(l - 1, k)\) for \(0 \leq k \leq a\). For \(x \in I\) and \(k \leq a\) we have

\[
\phi(x, k) = \phi(l - 1, k) + \sum_{n \in I, n \leq x \atop (n, n_k) = 1} f(n).
\]

Say we have a zero-based array

\[
f_{\text{block}} = [f(l + 0), f(l + 1), \ldots, f(l + B - 1)].
\]

Then for \(k\) from 0 to \(a\) we know that

\[
\phi(x, k) = \phi(l - 1, k) + \sum_{i = 0}^{x - l} f_{\text{block}}[i],
\]

and after we have calculated all the \(\phi\) values we need, we “strike out” the multiples of \(p_k\), i.e. setting \(f_{\text{block}}[i]\) to zero for \(p_k \mid l + i\), and proceed to the next \(k\).

Thankfully, there is an efficient data structure for calculating prefix sums of the mutable array: the Fenwick tree. Thus we may assume that this can be done efficiently.

For a special leaf \((n, b)\) we have \(n > Y\) and \(x/n < x/Y\). We will sieve interval \([1, x/Y]\) in blocks of size \(B\)

\[
I_k = [1 + (k - 1)B, 1 + kB) = [1 + (k - 1)B, kB],
\]

with the last block potentially shortened.

Since \(n = n^*p_{b+1}\), we can process this leaf after we have sieved the first \(b\) primes. Thus we get bounds

\[
\frac{x}{((k + 1)B + 1)p_{b+1}} < n^* \leq \frac{x}{(kB + 1)p_{b+1}},
\]

and

\[
n^* \in \left(\frac{x}{((k + 1)B + 1)p_{b+1}}, \frac{x}{(kB + 1)p_{b+1}}\right) \cap [1, Y],
\]

such that \(l_p(n^*) > p_{b+1}\), and \(\mu(n^*) \neq 0\).

We recall that a special node \((n, b)\) is such that \((n, P) = 1\), thus for the first \(K\) primes we only need to “strike out” their multiples; all this machinery is needed only starting with \(b = K + 1\). We can even reuse sieving results obtained from the precalculation of \(\phi\), if this proves efficient.
Now, we proceed to lower the number of primes considered per block, from the first \(a\) primes to the first \(\pi(\sqrt[3]{x})\) primes. Following [1] we should further split special leaves. We will consider the 3 leaf classes:

1. \(\sqrt[3]{x} < l_p(n) \leq Y\)
2. \(\sqrt[3]{x} < l_p(n) \leq \sqrt[3]{x}\)
3. \(l_p(n) \leq \sqrt[3]{x}\)

We also note that if we use the precomputed \(\phi\) table, the special leaves \((n, b)\) must have \(b > K\). We might tweak lower bounds in the above, but this is way too complicated. It is way easier to either lower \(K\) to have \(K < \pi(\sqrt[3]{x})\) or to compute \(F(x)\) directly (as \(x\) is quite low in this case).

First of all we note that for \(n\) such that \(l_p(n) > \sqrt[3]{x}\), we must have \(n^*\) prime. Indeed, since \(l_p(n) > \sqrt[3]{x}\), for \(n^*\) not prime we immediately obtain

\[n^* > l_p(n)^2 > \sqrt[3]{x} > Y,\]

which contradicts the choice of \(n^*\). On the other hand, for any \(n^*\) prime we have

\[n = n^* l_p(n) > l_p(n)^2 > Y,\]

giving us a special leaf.

Thus the leaves of the first two kinds are of the form \(n = pq > Y\), with \(\sqrt[3]{x} < p < q \leq Y\), with their contribution being

\[
\sum_{\sqrt[3]{x} < p \leq Y} \sum_{p < q \leq Y} \mu(pq)f(pq)\phi\left(\frac{x}{pq}, \pi(p) - 1\right)
= \sum_{\sqrt[3]{x} < p \leq Y} f(p) \sum_{p < q \leq Y} f(q)\phi\left(\frac{x}{pq}, \pi(p) - 1\right).
\]

**4.3. Special Leaves I.** For \(\sqrt[3]{x} < p < q \leq Y\) we immediately notice that

\[pq > \sqrt[3]{x^2}, \text{ and } \frac{x}{pq} < \sqrt[3]{x} < p,\]

thus \(\phi\left(\frac{x}{pq}, \pi(p) - 1\right) = 1\). Their contribution is then

\[
S_{el} = \sum_{\sqrt[3]{x} < p \leq Y} f(p) \sum_{p < q \leq Y} f(q)
= \sum_{\sqrt[3]{x} < p \leq Y} f(p) \left(F(Y) - F(p)\right)
= F(Y) \sum_{\sqrt[3]{x} < p \leq Y} f(p) - \sum_{\sqrt[3]{x} < p \leq Y} f(p)F(p)
= F(Y) \left(F(Y) - F(\sqrt[3]{x})\right) - \sum_{\sqrt[3]{x} < p \leq Y} f(p)F(p),
\]

and we can compute this immediately after sieving \([1, Y]\)
4.4. **Special Leaves II.1.** Now we consider the leaves with $\sqrt[3]{x} < p \leq \sqrt[3]{x}$, and $q > x/p^2$. This gives us $p^2 > x/q \geq x/y$, and $\frac{x}{pq} < p$. Thus we have again $\phi \left( \frac{x}{pq}, \pi(p) - 1 \right) = 1$, so their contribution is

$$S_{c21} = \sum_{\sqrt[3]{Y} < p \leq \sqrt[3]{x}} f(p) \sum_{\sqrt[3]{Y} < q \leq Y} f(q)$$

$$= \sum_{\sqrt[3]{Y} < p \leq \sqrt[3]{x}} f(p) \left( F(Y) - F \left( \frac{x}{p^2} \right) \right)$$

$$= F(Y) \left( F(\sqrt[3]{x}) - F \left( \frac{\sqrt[3]{x}}{Y} \right) \right) - \sum_{\sqrt[3]{Y} < p \leq \sqrt[3]{x}} f(p) F \left( \frac{x}{p^2} \right).$$

Since $x/p^2 \leq Y$, we may assume that $F(x/p^2)$ was precomputed.

4.5. **Special Leaves II.2.** We consider the leaves with $\sqrt[3]{x} < p \leq \sqrt[3]{x}$, and $q \leq x/p^2$. For $\phi \left( \frac{x}{pq}, \pi(p) - 1 \right)$ we want the terms not divisible by primes below $p$, and we have $p < \frac{x}{pq} < \sqrt[3]{x} < p^2$. Thus the terms we want are exactly 1 and the prime numbers in the interval $[p, \frac{x}{pq}]$, giving us

$$\phi \left( \frac{x}{pq}, \pi(p) - 1 \right) = 1 + \sum_{\substack{p \leq r \leq \frac{x}{pq} \atop r \text{ prime}}} f(r)$$

$$= 1 + F \left( \frac{x}{pq} \right) - F(p) - 1.$$ 

Thus the total contribution of these nodes is

$$S_{c22} = \sum_{\sqrt[3]{Y} < p \leq \sqrt[3]{x}} f(p) \sum_{p < q \leq \min \left( \sqrt[3]{Y}, \sqrt[3]{x/p^2} \right)} f(q) \left( 1 + F \left( \frac{x}{pq} \right) - F(p) - 1 \right)$$

$$= \sum_{\sqrt[3]{Y} < p \leq \sqrt[3]{x}} f(p) \left( 1 - F(p) - 1 \right) \sum_{p < q \leq \min \left( \sqrt[3]{Y}, \sqrt[3]{x/p^2} \right)} f(q)$$

$$+ \sum_{\sqrt[3]{Y} < p \leq \sqrt[3]{x}} f(p) \sum_{p < q \leq \min \left( \sqrt[3]{Y}, \sqrt[3]{x/p^2} \right)} f(q) F \left( \frac{x}{pq} \right).$$
We note, that \( Y \leq x/p^2 \) when \( p^2 \leq x/Y \). We start by using this to split the first sum above into the sums without conditions:

\[
\sum_{\sqrt{Y}<p \leq \sqrt{Y}/Y} f(p) (1 - F(p-1)) \sum_{p < q \leq Y} f(q) \quad \text{and} \quad \sum_{\sqrt{Y}/Y < p \leq \sqrt{Y}} f(p) (1 - F(p-1)) \sum_{p < q < x/p^2} f(q) \end{equation}
\]

That gives us

\[
\sum_{\sqrt{Y}<p \leq \sqrt{Y}/Y} f(p) (1 - F(p-1)) \sum_{p < q \leq \min(x/p^2,Y)} f(q) = V_1 + V_2 - V_3,
\]

with

\[
V_1 = \sum_{\sqrt{Y}<p \leq \sqrt{Y}/Y} f(p) (1 - F(p-1)) \quad F(Y)
\]

\[
= F(Y) \sum_{\sqrt{Y}<p \leq \sqrt{Y}/Y} f(p) (1 - F(p-1))
\]

\[
= F(Y) \left( F \left( \sqrt{\frac{x}{Y}} \right) - F \left( \sqrt{\frac{x}{Y}} \right) \right) - F(Y) \sum_{\sqrt{Y}<p \leq \sqrt{Y}/Y} f(p)F(p-1)
\]

\[
V_2 = \sum_{\sqrt{Y}/Y < p \leq \sqrt{Y}} f(p) (1 - F(p-1)) F \left( \frac{x}{p^2} \right)
\]

\[
= \sum_{\sqrt{y}/Y < p \leq \sqrt{Y}} f(p)F \left( \frac{x}{p^2} \right) - \sum_{\sqrt{y}/Y < p \leq \sqrt{Y}} f(p)F(p-1)F \left( \frac{x}{p^2} \right)
\]

\[
V_3 = \sum_{\sqrt{Y}<p \leq \sqrt{Y}/Y} f(p) (1 - F(p-1)) F(p)
\]

\[
= \sum_{\sqrt{Y}<p \leq \sqrt{Y}/Y} f(p)F(p) - \sum_{\sqrt{Y}<p \leq \sqrt{Y}/Y} f(p)F(p-1)F(p)
\]

As before we note that all the values of \( F \) has the argument in \([1,Y]\).

We proceed similarly for the second sum:

\[
\sum_{\sqrt{Y}<p \leq \sqrt{Y}/Y} f(p) \sum_{p < q \leq \min(x/p^2,Y)} f(q) F \left( \frac{x}{pq} \right) = W_1 + W_2,
\]
where

\[ W_1 = \sum_{\sqrt{x/p} \leq \sqrt{Y}} f(p) \sum_{p < q \leq Y} f(q)F\left(\frac{x}{pq}\right) \]

\[ W_2 = \sum_{\sqrt[3]{x/Y} \leq p \leq \sqrt{x}} f(p) \sum_{p < q \leq \sqrt{x/p^2}} f(q)F\left(\frac{x}{pq}\right) \]

We note that we can proceed in a similar way to the calculation of \( P_2 \): as we sieve the block, for primes \( p \in (\sqrt{x}, \sqrt[3]{x}) \) we find bounds on \( q \), so that \( F\left(\frac{x}{pq}\right) \) is in the current block. Noting that \( q \leq \sqrt{x} \), unlike \( P_2 \), we do not need to sieve the resulting interval. Further, \( \sqrt[3]{x/p^2} \leq \sqrt{x} \), give us the upper bound on blocks we need to consider.

### 4.6. Special Leaves: Bringing it all together.

As we have seen above, all the terms in \( S_{c1}, S_{c21}, \) and \( V_1, V_2, V_3 \) can be precomputed. We should try to combine these sums. First of all, the constant term is

\[
F(Y) \left( F(Y) - F(\sqrt{x}) \right) + F(Y) \left( F(\sqrt{x}) - F\left(\sqrt{\frac{x}{Y}}\right) \right) + F(Y) \left( F\left(\sqrt{\frac{x}{Y}}\right) - F(\sqrt[3]{x}) \right)
\]

Then we combine the terms involving \( f(p)F(p) \) to get: \( - \sum_{\sqrt{x} < p \leq \sqrt{Y}} f(p)F(p) \). Further, the terms involving \( f(p)F(\sqrt{x}) \) are annihilated.

Thus

\[
S_1 = S_{c1} + S_{c21} + V_1 + V_2 + V_3
\]

\[
= F(Y) \left( F(Y) - F(\sqrt{x}) \right) - \sum_{\sqrt{x} < p \leq \sqrt{Y}} f(p)F(p)
\]

\[
- F(Y) \sum_{\sqrt{x} < p \leq \sqrt{Y}} f(p)F(p - 1)
\]

\[
- \sum_{\sqrt[3]{x/Y} < p \leq \sqrt{x}} f(p)F(p - 1)F\left(\frac{x}{p^2}\right)
\]

\[
+ \sum_{\sqrt{x} < p \leq \sqrt[3]{x}} f(p)F(p - 1)F(p)
\]

and, as noted above, all the values used can be computed once \([1, Y]\) is sieved.

We set \( S_2 = W_1 + W_2 \), which should be updated per-block in \([1, \sqrt{x}]\). And we set \( S_3 \) to be the contribution of the special leaves of the third class, which should use the algorithm described above to update the values of \( \phi \).
Thus, to summarize:

1. We calculate the contribution of ordinary leaves.
2. We calculate $S_1$.
3. For each block in $[1, \sqrt{x}]$ we update $S_2$.
4. For each block we update the table of $\phi(n, b)$ for $b \leq \sqrt{x}$ and use it to calculate $S_3$.

For $S_1$ we note that, to allocate less memory, all the terms apart from the sum of $f(p)F(p-1)F(\pi/p^2)$ can be calculated per block. And for the latter we need to only store $F(p-1)$ for primes in $\left(\sqrt{x}/\sqrt{y}, \sqrt{x}\right)$, noting that this will be available before we calculate $F(\pi/p^2)$, so we can, again, calculate this sum per-block.

We can lessen the memory usage further. Note that $p \leq \pi/p^2$. Suppose we have calculated $F(p-1)$ for the largest $p$ not greater than $\sqrt{x}$. Afterwards we will encounter the values $\pi/p^2$ in the order of $p$ descending; thus after processing $p_k$ we subtract $f(p_{k-1})$ from the accumulator and continue.

5. Parallelizing Computations

We note that a lot of computations can be easily parallelized. We start with $P_2$ computation.

5.1. Computation of $P_2$. As before, we proceed in blocks $I = [l, l+B)$. Let’s write $F_I$ for “in block” sumatory function of $f$, i.e. $F_I(x) = \sum_{l \leq p < x} f(p)$, assuming $x \in I$. Then the contribution of $I$ into $S_2$ would be

$$S_{2I} = \sum_{l \leq p < l+B} f(p)F(p-1) = \sum_{l \leq p < l+B} f(p)(F(l-1) + F_I(p-1))$$

$$= F(l-1) \sum_{l \leq p < l+B} f(p) + \sum_{l \leq p < l+B} f(p)F_I(p-1).$$

Thus to compute $S_2$ in parallel, we split it into two parts: first of all we sum the values of $\sum_{l \leq p < l+B} f(p)F_I(p-1)$ per block, and also we compute $F_I(l+B-1)$ per block. The latter values can be used to reconstruct $F(l-1)$ in order.

We proceed similarly for $S_1$

$$S_{1I} = \sum_{l \leq \pi/p < l+B} f(p)F\left(\frac{x}{p}\right) = \sum_{l \leq \pi/p < l+B} f(p)\left(F(l-1) + F_I\left(\frac{x}{p}\right)\right)$$

$$= F(l-1) \sum_{l \leq \pi/p < l+B} f(p) + \sum_{l \leq \pi/p < l+B} f(p)F_I\left(\frac{x}{p}\right),$$

and once again, the second sum is fully computed per block, and the first one is reconstructed.

5.2. Computation of $\phi$. For $S_1$ we note that we have sums involving products $F(p-1)F(\pi/p^2)$ and $F(p-1)F(p)$ which is hard to handle in the same manner as above. Thus we should handle it separately, either by going in blocks through $[1, Y]$, or, as we sieve $[1, Y]$ anyway, we can precompute all the values of $F(n)$ in this interval and then run in blocks in parallel, as then we won’t have any
interdependency.
For $S_2$ we proceed similar to the calculation of $P_2$:

$$S_{2I} = \sum_{x/\ pq \in I} f(p)f(q)F\left(\frac{x}{pq}\right) = \sum_{x/\ pq \in I} f(p)f(q) \left[ F(l-1) + F_1\left(\frac{x}{pq}\right) \right]$$

$$= F(l-1) \sum_{x/\ pq \in I} f(p)f(q) + \sum_{x/\ pq \in I} f(p)f(q)F_1\left(\frac{x}{pq}\right).$$

For $S_3$ we write

$$G_I(x, k) = \sum_{n \in I, n \leq x} f(n), \quad g(n, b) = \mu(n)f(n)f(p^{b+1}),$$

and we have

$$S_{3I} = - \sum_{x/\ n^*p_{b+1} \in I} g(n^*, p_{b+1}) \left[ \phi(l-1, b) + G_I\left(\frac{x}{n^*p_{b+1}}, b\right) \right]$$

$$= - \sum_{b} \phi(l-1, b) \sum_{x/\ n^*p_{b+1} \in I} g(n^*, p_{b+1}) - \sum_{x/\ n^*p_{b+1} \in I} g(n^*, p_{b+1})G_I\left(\frac{x}{n^*p_{b+1}}, b\right).$$

We note that we touch only "trivial" parallelization concerns. We refer to [6] for an in-deep discussion of the possible optimizations, as here we are mostly interested in maths.

6. Computational Analysis

As we do the analysis to find the guidelines to select the good values for $Y$ and $B$, we should ignore the impact of the multi-precision arithmetic (if it is used), so we assume that multiplications, additions and the calculation of $f$ is $O(1)$.

6.1. Cost of Sieving. Our main subtask will be to sieve the interval of length $N$ with primes up to $Y$. The complexity can be estimated as

$$N \sum_{p \leq Y} \frac{1}{p} \sim N \log \log Y.$$  

We start with sieving $[1, Y]$, and then we fully sieve $[Y, x/y]$ in blocks of size $B$ using only primes up to $Y$. The total complexity of the sieving step is then

$$O \left(\frac{x}{Y} \log \log Y\right).$$

6.2. Cost of $P_2$. For $S_1$ we need to sieve disjoint subintervals of $[\sqrt{x}, x/y]$ to find $q$ for $x/q$ to be in the current block. We may estimate this as the time to fully sieve $[\sqrt{x}, x/y]$ giving us

$$O \left(\frac{x}{Y} \log \log Y\right).$$

Then we sum $\pi(\sqrt{x}) - \pi(Y)$ terms giving us an estimate of

$$O \left(\pi(\sqrt{x}) - \pi(Y)\right) = O \left(\frac{\sqrt{x}}{\log x}\right).$$
Since $\sqrt{x} \leq x/y$ we have the cost of $P_2$ to be $$O \left( \frac{x}{Y} \log \log Y \right).$$

6.3. Cost of $\phi$: $S_1$. In here we have simple sums, so the total complexity depends just on the number of terms, and can be approximated by $$O(\pi(Y)) = O \left( \frac{Y}{\log Y} \right).$$

6.4. Cost of $\phi$: $S_2$. To estimate the complexity of computing $W_1$ we need to count the number of terms in the sum. This gives us

$$\left( \pi(Y) - \pi \left( \sqrt[3]{x} \right) \right) + \cdots + \left( \pi(Y) - \pi \left( \sqrt[4]{x} \right) \right)$$

$$= \frac{\pi \left( \sqrt[3]{x} \right) - \pi \left( \sqrt[4]{x} \right)}{2} \left[ 2\pi(Y) - \left( \pi \left( \frac{x}{Y} \right) + \pi \left( \sqrt[3]{x} \right) \right) \right]$$

First of all we note that $\sqrt[3]{x} \leq Y < \sqrt[3]{x}$ hence we have

$$\sqrt[3]{x} < \sqrt[3]{\frac{x}{y}} \leq \sqrt[3]{x}.$$ 

Thus the sum above can be approximated by

$$O \left( \frac{Y \sqrt[3]{x}}{\log^2 x} \right).$$

Similarly for $W_2$ we have $\sqrt[3]{x} \leq x/p^2 < Y$ and

$$O \left( \sum_{\sqrt[3]{y}/p \leq \sqrt[3]{x}} \pi \left( \frac{x}{p^2} \right) \right) = O \left( \pi \left( \sqrt[4]{x} \right) \right) O \left( \pi \left( Y \right) \right) = O \left( \frac{Y \sqrt[4]{x}}{\log^2 x} \right).$$

6.5. Cost of $\phi$: $S_3$. The process of sieving blocks is made complicated here by the Fenwick Tree. For each node of interest we need to calculate the prefix sum, giving us $O(\log B)$ complexity. To estimate the number of the nodes we need to process we note that they have form $(n^* p_{b+1}, b)$ with $n^* \leq Y$ and $b \leq \pi \left( \sqrt[4]{x} \right)$, giving us a total of

$$O \left( Y \pi \left( \sqrt[4]{x} \right) \log B \right).$$

Also, we need to account for updating the Fenwick tree. We note that we touch every value at most once: first time when we initialize the tree for a block, and a second time when we “strike out” this value\(^1\), thus giving us an estimation on the extra work to be

$$O \left( \frac{x}{Y} \log B \right).$$

\(^1\)We should note that this is a very crude estimation as we strike out the multiples of the first $K$ primes without any extra processing.
6.6. **Total Cost.** We see that the total cost is about

\[ O \left( \frac{x}{Y} \log \log Y + \frac{Y}{\log Y} + \frac{Y \sqrt{x}}{\log^3 x} + \frac{x}{Y} \log B + \frac{Y \sqrt{x} \log B}{\log x} \right). \]

Ignoring \( B \) for now (we can approximate it with \( \log B \approx \log Y \)) we note that setting \( Y = O (\sqrt[3]{3x \log 3x}) \) will give us the total estimate of

\[ O \left( \frac{x^{3/4}}{\log^2 x} \right). \]

Following [7] we should set \( Y = \alpha \sqrt{x} \) with

\[ \alpha = a \log^3 x + b \log^2 x + c \log x + d, \]

and find the optimal values for \( a, b, c, d \) empirically.

6.7. **Finding \( \alpha \).** As noted in [5], “changes of \( \pm 25\% \) around the optimal value of \( \alpha \) did not increase the execution time by more than 3\%”, which agrees with our experiments. Thus for a given \( x \) we fix the interval \([\alpha_0, \alpha_1]\) and calculate \( F(x) \) using a different \( \alpha \), finding the one that gives us the fastest running time. We repeat this for several values of \( x \) and then we find the best fitting values. We must say that this process is pretty “noisy” thus we did several runs of it. Even then, from our experiments, the optimal value of \( \alpha \) does not change considerably with changing the power exponent, thus we can have one formula to calculate \( \alpha \) for all. The results we’ve got on the author’s computer are as follows:

| \( x \)    | \( 10^3 \) | \( 10^4 \) | \( 5 \times 10^4 \) | \( 10^5 \) | \( 5 \times 10^5 \) | \( 10^6 \) | \( 5 \times 10^6 \) | \( 10^7 \) | \( 5 \times 10^7 \) | \( 10^8 \) |
|----------|-----------|-----------|-----------------|-----------|-----------------|-----------|-----------------|-----------|-----------------|-----------|
| \( \alpha \) | 3         | 3.5       | 5               | 6         | 7               | 8         | 8.5             | 10        | 12              | 13        |

Fitting the values to the data we obtain the formula

\[ \alpha \approx 0.000681 \log x^3 - 0.011846 \log x^2 + 0.044074 \log x + 0.988365. \]

7. **Numerical Results**

We give some values of the function \( F_n(x) = \sum_{p \leq x} p^n \).

We have checked the correctness of our algorithms in several ways. First of all, for \( n = 0 \) and \( n = 1 \) we have compared the results to the known values: for \( n = 0 \) Wikipedia has an extensive table and for \( n = 1 \) we have used the values from [7]. For “smaller” values of \( x \) we have checked the results against Pari/GP. We have also computed \( F_n(x) \) and \( F_n(x + \varepsilon) \), and checked that these agree by sieving \([x, x + \varepsilon]\) and calculating the value of \( F_n(x + \varepsilon) \) from \( F_n(x) \) and now known primes. We have also tested extensively for the small \( x \), using the variation of parameters: \( Y, B \), and \( K \).

We note that we have used 256-bit arithmetics for our calculations, so the table for \( F_4(x) \) is shorter due to overflows with larger values of \( x \).
Table 1. Values of $F_2(x)$

| $10^{10}$ | 14692485666215945973239505690 |
| 5 $\times$ $10^{10}$ | 171486303117140782670294223341 |
| $10^{11}$ | 13338380640732671147186590712800 |
| 5 $\times$ $10^{11}$ | 15663981441957803298126641928041 |
| $10^{12}$ | 122129079617761747436156085876997 |
| 5 $\times$ $10^{12}$ | 144159398892141564900337100187358316 |
| $10^{13}$ | 1126261785640702236670513970349205634 |
| 5 $\times$ $10^{13}$ | 13352101252957702984731843412618920082018 |
| $10^{14}$ | 10449549945144268110573967892555485354493 |
| 5 $\times$ $10^{14}$ | 1243450253668811479272045017247069947749359 |
| $10^{15}$ | 9745981795365753183493378490092915742101696 |
| 5 $\times$ $10^{15}$ | 1163492503926172589836028218116001190925369911 |
| $10^{16}$ | 91311874198611609023464503082745094925133348 |
| 5 $\times$ $10^{16}$ | 1093197297594496716923810873727618016729821706326 |
| $10^{17}$ | 8593608224398905676209125328673103991944617500636 |

Table 2. Values of $F_3(x)$

| $10^{10}$ | 10978000188533601058523979120755908 |
| 5 $\times$ $10^{10}$ | 640820468207234514870756138899001998582245 |
| $10^{11}$ | 996973732171667396998099396013424430102364 |
| 5 $\times$ $10^{11}$ | 585520088966490975269979571553990313510861 |
| $10^{12}$ | 9131183180200496139738672227721825939508051079 |
| 5 $\times$ $10^{12}$ | 539011223765053862349869931020562476048206694122 |
| $10^{13}$ | 842276414261296966546399463495855318856709486404 |
| 5 $\times$ $10^{13}$ | 499344581758773303056840568583752148579098600691128 |
| $10^{14}$ | 78163576831397402977652927326003337487234114404747147 |
| 5 $\times$ $10^{14}$ | 465116388359752429200756526955719292849606973899669709221 |
| $10^{15}$ | 729140872559557278292350232663571878326704107244928337284 |
| 5 $\times$ $10^{15}$ | 435279828236658213739213157789526698543063668255079308939 |
| $10^{16}$ | 68325370067325544708478272449701292580760449875092937488310 |
| 5 $\times$ $10^{16}$ | 4099406064764055185674494652258362155343639276731729319850 |
| $10^{17}$ | 642800454307687984344682304535086826246739426032801572692032867900 |
**Table 3. Values of $F_4(x)$**

| $x$  | $10^{10}$                                      | $5 \times 10^{10}$                             | $10^{11}$                                      | $5 \times 10^{11}$                             | $10^{12}$                                      | $5 \times 10^{12}$                             | $10^{13}$                                      | $5 \times 10^{13}$                             | $10^{14}$                                      | $5 \times 10^{14}$                             | $10^{15}$                                      |
|------|------------------------------------------------|------------------------------------------------|------------------------------------------------|------------------------------------------------|------------------------------------------------|------------------------------------------------|------------------------------------------------|------------------------------------------------|------------------------------------------------|------------------------------------------------|------------------------------------------------|
| $10^{10}$ | 876279913324387539183894015044723229219045342750 | $255793553749495874075950241776379969239226020428977$ | $79596284512301003834661995024051166148172171338371852$ | $233763531449591824849643583298329925979435007893090787181$ | $7291405674369073009761776122154275329527216556249514408897$ | $2152273506368350599911726874815472855602976344249380004455248$ | $672670357329861006491888367274980639337624917176989202367080838$ | $1994144875417964028004350412269602745929105301922832366911602292806$ | $624318568918260599532308267428384030203995668819924057075933466801$ | $185766273878955147609467369321682910437837624744901019253719657653093899$ | $5824519129976593880511325120158491808935524746219691118247177308917094908$ |
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