

COMPUTING $\pi(x)$ ANALYTICALLY

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ABSTRACT. We describe a rigorous implementation of the Lagarias and Odlyzko Analytic Method to evaluate the prime counting function and its use to compute unconditionally the number of primes less than 10^{24} .

1. INTRODUCTION

Computing exact values of the function $\pi(x)$, which counts the number of primes less than or equal to x , has exercised mathematicians since antiquity. Early methods involved enumerating all the primes less than the target x (using, for example, the sieve of Eratosthenes) and then counting them. In 1870 Meissel [12] described a combinatorial method which he eventually used to manually compute $\pi(10^9)$ [13] (albeit not quite accurately). The algorithm was subsequently improved by Lehmer [11], then by Lagarias, Miller and Odlyzko [10] and most recently by Deléglise and Rivat [7]. In 2007 Oliveira e Silva used the algorithm to compute $\pi(10^{23})$.

The Prime Number Theorem dictates that all methods reliant on enumerating the primes must have time complexity of $\Omega(x \log^{-1} x)$. The latest incarnations of the combinatorial method achieve $\mathcal{O}(x^{2/3} \log^{-2} x)$.

In their 1987 paper [9], Lagarias and Odlyzko described an analytic algorithm with (in one form) time complexity $\mathcal{O}(x^{1/2+\epsilon})$. In 2010 Büthe, Franke, Jost and Kleinjung announced a value for $\pi(10^{24})$ [5] contingent on the Riemann Hypothesis. Their approach “is similar to the one described by Lagarias and Odlyzko, but uses the Weil explicit formula instead of complex curve integrals”. This paper describes an implementation reverting to Riemann’s explicit formula which we have used to compute $\pi(10^{24})$ unconditionally.

2. A NOTE ON RIGOUR

To many, rigorous computation is an oxymoron, due to potential bugs in hardware, operating systems, compilers and (most likely) the user’s code. Add to this the chance that a power spike or cosmic ray interaction could scupper even a correctly written application, and the situation seems hopeless. We do what we reasonably can to minimise such risks including running applications on systems with ECC memory after testing on hardware from different vendors with different operating systems and using different compilers.

However, there are certain aspects over which we do have more control. Estimating the rounding error that will accumulate through a complex floating point

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computation is a non-trivial task that we eschew. Rather, we rely on interval arithmetic (see [14] for a good introduction). Thus, instead of storing a single floating point approximation, we hold an interval comprising two floating points to bracket the true value. We then overload the standard operators and functions to handle such intervals.

Furthermore, we will estimate some quantities by, for example, truncating an infinite sum. We will need to derive a rigorous bound for the error introduced, but rather than keep track of such errors manually, we can simply add them to the interval being evaluated and let the software take over. Indeed, we can in some circumstances use interval arithmetic to compute such bounds for us.

3. THE ANALYTIC ALGORITHM

The analytic algorithm relies on Perron's formula.

Theorem 3.1 (Perron's formula). *Let $a(n)$ be an arithmetic function with Dirichlet series*

$$g(s) = \sum_{n=1}^{\infty} \frac{a(n)}{n^s}.$$

Now if $g(s)$ is absolutely convergent whenever $\Re s > \sigma_a$, then for $c > \sigma_a$ and $x > 0$ we have

$$\sum_{n \leq x}^* a(n) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} g(s) x^s \frac{ds}{s},$$

where the $$ on the summation sign indicates that if x is an integer, then only $1/2$ of the $a(x)$ term is included.*

Proof. See page 245 of [1] and the subsequent note. □

The relevance of Perron's formula to the matter at hand comes from the series, absolutely convergent for $\Re s > 1$,

$$\log \zeta(s) = \sum_{n=2}^{\infty} \frac{\Lambda(n)}{n^s \log n}.$$

Here Λ is the von Mangoldt function so $\frac{\Lambda(n)}{\log n}$ is $\frac{1}{m}$ at prime powers p^m and zero elsewhere. Define

$$\pi^*(x) := \sum_{p^m \leq x} \frac{1}{m},$$

where if x is a prime power we only take $1/2$ of its contribution to the sum. Then applying Perron's formula we get for $c > 1$ and $x > 0$

$$(3.1) \quad \sum_{n \leq x}^* \frac{\Lambda(n)}{\log n} = \pi^*(x) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} \log \zeta(s) x^s \frac{ds}{s}.$$

Here we note that, although we can cheaply recover $\pi(x)$ from $\pi^*(x)$, the slow rate of convergence of the integral dooms any attempt to use it in this context.

At this point, Lagarias and Odlyzko introduce a “suitable” Mellin transform pair $\phi(t)$ and $\hat{\phi}(s)$ and derive

$$(3.2) \quad \pi^*(x) = \frac{1}{2\pi i} \int_{\sigma-i\infty}^{\sigma+i\infty} \log \zeta(s) \hat{\phi}(s) ds + \sum_{p^m} \frac{1}{m} [\chi_x(p^m) - \phi(p^m)],$$

where $\chi_x(t)$ is defined by

$$\chi_x(t) := \begin{cases} 1, & t < x, \\ 1/2, & t = x, \\ 0, & t > x. \end{cases}$$

We note that taking $\hat{\phi}(s) = \frac{x^s}{s}$ makes $\phi(t) = \chi_x(t)$ and we recover (3.1).

Thus estimating $\pi^*(x)$ now splits into estimating an integral and summing $\phi(t)$ evaluated at prime powers in the vicinity of x .

In his PhD thesis [8] Galway investigated the proposed algorithm and suggested using the Mellin transform pair

$$(3.3) \quad \hat{\phi}(s) := \frac{x^s}{s} \exp\left(\frac{\lambda^2 s^2}{2}\right) \text{ and } \phi(t) := \frac{1}{2} \operatorname{erfc}\left(\frac{\log\left(\frac{t}{x}\right)}{\sqrt{2}\lambda}\right).$$

Here erfc is the complementary error function

$$\operatorname{erfc}(x) := \frac{2}{\sqrt{\pi}} \int_x^\infty \exp(-t^2) dt$$

and λ is a positive real parameter used to balance the convergence of the integral with the width of the prime sieve.

Galway showed that ϕ and $\hat{\phi}$ as defined in (3.3) are indeed “suitable” and, using arguments based on the uncertainty principle, suggested that they are in some sense optimal. He also gave a rigorous bound for the error introduced by truncating the prime sieve to some finite width.

4. EVALUATING $\frac{1}{2\pi i} \int_{\sigma-i\infty}^{\sigma+i\infty} \log \zeta(s) \hat{\Phi}(s) Ds$

At this point, we depart from the line taken by Lagarias and Odlyzko. Rather than attempt to numerically estimate the integral in (3.2), we take an approach closer to the spirit of Riemann and evaluate it in terms of the non-trivial zeros of ζ , leading to Theorem 4.7 below.

Before proceeding, we need a couple of lemmas.

Lemma 4.1. *The “Round the Pole” lemma. Let f be a meromorphic function with a simple pole at α with residue R , and let Γ be the semicircular contour counter-clockwise from $\alpha + \epsilon$ to $\alpha - \epsilon$. Then*

$$\lim_{\epsilon \rightarrow 0^+} \int_{\Gamma} f(z) dz = \pi i R.$$

Proof. See page 29 of [18]. □

Lemma 4.2. *We have*

$$\lim_{\epsilon \rightarrow 0^+} (\log \zeta(1 + \epsilon) - \log(-\zeta(1 - \epsilon))) = 0.$$

Proof.

$$\begin{aligned} \lim_{\epsilon \rightarrow 0^+} (\log \zeta(1 + \epsilon) - \log(-\zeta(1 - \epsilon))) &= \lim_{\epsilon \rightarrow 0^+} \log \frac{\zeta(1 + \epsilon)}{-\zeta(1 - \epsilon)} \\ &= \lim_{\epsilon \rightarrow 0^+} \log \frac{1/\epsilon + \mathcal{O}(1)}{1/\epsilon + \mathcal{O}(1)} = 0. \quad \square \end{aligned}$$

Lemma 4.3. *There exists a sequence of $T_j \rightarrow \infty$ such that for any $\sigma \in [-1, 2]$ we have for $s = \sigma + iT_j$*

$$\frac{\zeta'}{\zeta}(s) = \mathcal{O}(\log^2 T_j).$$

Proof. Referring to Davenport [6], for any zero $\beta + i\gamma$ of ζ with γ large, we note that there are $\mathcal{O}(\log \gamma)$ zeros with imaginary part $\in [\gamma - 1, \gamma + 1]$ (Corollary (a), page 99). Therefore we can select a T_j within $\mathcal{O}(1)$ of γ such that T_j differs from the imaginary part of any zero by $\gg \frac{1}{\log T_j}$. By (4) on page 99 we have for $\sigma \in [-1, 2]$

$$\left| \frac{\zeta'}{\zeta}(\sigma + iT_j) \right| = \left| \sum_{\rho}' \frac{1}{\sigma + iT_j - \rho} + \mathcal{O}(\log T_j) \right|,$$

where the sum is taken over zeros with imaginary part $\in [T_j - 1, T_j + 1]$. There are $\mathcal{O}(\log T_j)$ such zeros, each one making a contribution to the sum limited by $\mathcal{O}(\log T_j)$ and the result follows. \square

Lemma 4.4. *For $t \in \mathbb{R}$*

$$|\log(-\zeta(-1 + it))| \leq 5 + t^2.$$

Proof. By the functional equation

$$\zeta(-1 + it) = \zeta(2 - it) \frac{\Gamma\left(\frac{2 - it}{2}\right)}{\Gamma\left(\frac{-1 + it}{2}\right)} \pi^{(-\frac{3}{2} + it)}.$$

We then use $\left(\frac{-1 + it}{2}\right) \Gamma\left(\frac{-1 + it}{2}\right) = \Gamma\left(\frac{1 + it}{2}\right)$ so we can apply Stirling's approximation. Also, for $\Re s > 1$ we have

$$|\log \zeta(s)| = \left| \sum_{n=2}^{\infty} \frac{\Lambda(n)}{\log(n)} \frac{1}{n^s} \right| \leq \sum_{n=2}^{\infty} \frac{\Lambda(n)}{\log(n)} \frac{1}{n^{\Re s}} = \log \zeta(\Re s). \quad \square$$

Lemma 4.5.

$$\left| \frac{1}{2\pi i} \int_{-1 - i\infty}^{-1 + i\infty} \log(-\zeta(s)) \widehat{\phi}(s) ds \right| \leq \frac{\exp\left(\frac{\lambda^2}{2}\right)}{2\pi x \lambda} \left(5\sqrt{2\pi} + \frac{2}{\lambda} \right).$$

Proof. We use Lemma 4.4 and take absolute values, majorising with

$$\frac{\exp\left(\frac{\lambda^2}{2}\right)}{2\pi x} \left[5 \int_{-\infty}^{\infty} \exp\left(\frac{-\lambda^2 t^2}{2}\right) dt + \int_{-\infty}^{\infty} |t| \exp\left(\frac{-\lambda^2 t^2}{2}\right) dt \right],$$

where both integrals can be evaluated. \square

Lemma 4.6. *Let $\widehat{\Phi}(s)$ be the unique holomorphic function $\widehat{\Phi} : \mathbb{C} \setminus \mathbb{R}_{\leq 0} \rightarrow \mathbb{C}$ such that*

- $\widehat{\Phi}'(s) = \widehat{\phi}(s)$ and
- $\lim_{t \rightarrow \infty} [\widehat{\Phi}(\sigma + it) + \widehat{\Phi}(\sigma - it)] = 0$ for any fixed real σ .

Then

- (1) $\widehat{\Phi}(s) - \log s$ extends to an entire function,
- (2) $\lim_{t \rightarrow \infty} \widehat{\Phi}(\sigma + it) = C$ is purely imaginary and
- (3) $\widehat{\Phi}(\sigma \pm it) \mp C$ is rapidly decreasing as $t \rightarrow \infty$.

Proof. To show (1) we define for $s \notin \mathbb{R}_{\leq 0}$

$$F(s) = \int_1^s \widehat{\phi}(z) dz,$$

where the contour of integration is the straight line from 1 to s . We then define

$$\widehat{\Phi}(s) := \lim_{T \rightarrow \infty} \left[F(s) - \frac{F(1 + iT) + F(1 - iT)}{2} \right]$$

and we have

$$F(s) - \log s = \int_1^s \left(\widehat{\phi}(z) - \frac{1}{z} \right) dz.$$

To show (2) we observe that $\widehat{\Phi}(\overline{s}) = \overline{\widehat{\Phi}(s)}$ and from the definition we have $C + \overline{C} = 0$.

To show (3), we take $T > 0$ and we have

$$|\widehat{\Phi}(\sigma \pm iT) \mp C| \leq \frac{x^\sigma}{T} \exp\left(\frac{\sigma^2 \lambda^2}{2}\right) \int_T^\infty \exp\left(\frac{-\lambda^2 t^2}{2}\right) dt. \quad \square$$

Theorem 4.7. *Let $\widehat{\Phi}(s)$ be defined as in Lemma 4.6. Then*

$$\frac{1}{2\pi i} \int_{2-i\infty}^{2+i\infty} \widehat{\phi}(s) \log \zeta(s) ds = \widehat{\Phi}(1) - \sum_{\rho} \Re \widehat{\Phi}(\rho) - \log(2) + \frac{1}{2\pi i} \int_{-1-i\infty}^{-1+i\infty} \widehat{\phi}(s) \log(-\zeta(s)) ds.$$

Proof. We will refer to the contours represented in Figure 1. These contours are:

- Γ_1 - the semi-circle clockwise from $1 - \epsilon$ to $1 + \epsilon$ for ϵ small and positive.
- Γ_2 - the semi-circle clockwise from $1 + \epsilon$ to $1 - \epsilon$.
- Γ_3 - the horizontal line from $1 + \epsilon$ to 2.
- Γ_4 - the horizontal line from 2 to $1 + \epsilon$.
- Γ_5 - the vertical line from 2 to $2 + iT_j$, T_j not the ordinate of a zero of ζ .
- Γ_6 - the vertical line from $2 - iT_j$ to 2.
- Γ_7 - the horizontal line from $2 + iT_j$ to $-1 + iT_j$.
- Γ_8 - the horizontal line from $-1 - iT_j$ to $2 - iT_j$.
- Γ_9 - the vertical line from $-1 + iT_j$ to $-1 + \frac{5}{4}i$, followed by the clockwise circular arc centred at -1 to $\frac{1}{4}$.
- Γ_{10} - the clockwise circular arc centred at -1 from $\frac{1}{4}$ to $-1 - \frac{5}{4}i$, followed by the vertical line to $-1 - iT_j$.
- Γ_{11} - the horizontal line from $\frac{1}{4}$ to $1 - \epsilon$.
- Γ_{12} - the horizontal line from $1 - \epsilon$ to $\frac{1}{4}$.

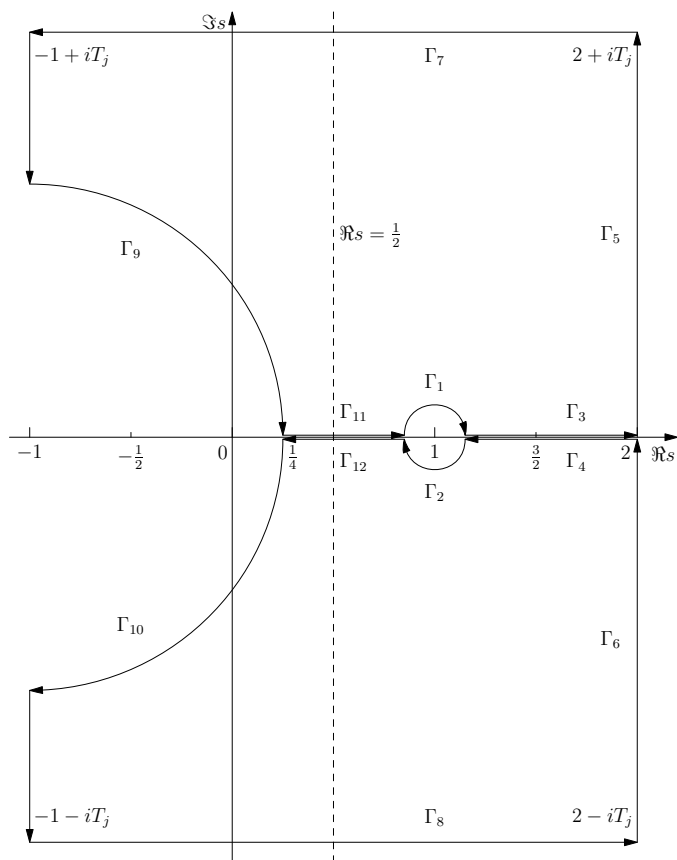


FIGURE 1. Contours to evaluate $\frac{1}{2\pi i} \int_{2-i\infty}^{2+i\infty} \hat{\phi}(s) \log \zeta(s) ds$

We consider the integrals

$$(4.1) \quad \frac{1}{2\pi i} \int (\hat{\Phi}(s) - C) \frac{\zeta'(s)}{\zeta(s)} ds$$

for the contours $\Gamma_1, \Gamma_3, \Gamma_5, \Gamma_7, \Gamma_9$ and Γ_{11} in the upper half plane and

$$(4.2) \quad \frac{1}{2\pi i} \int (\hat{\Phi}(s) + C) \frac{\zeta'(s)}{\zeta(s)} ds$$

for $\Gamma_2, \Gamma_4, \Gamma_6, \Gamma_8, \Gamma_{10}$ and Γ_{12} in the lower half.

We denote the integrals in (4.1) or (4.2) as appropriate along Γ_n by I_n and proceed as follows.

For I_5 and I_6 we get

$$\begin{aligned}
 \lim_{j \rightarrow \infty} (I_5 + I_6) &= \lim_{j \rightarrow \infty} \frac{1}{2\pi i} \left[\int_{\Gamma_5} (\widehat{\Phi}(s) - C) \frac{\zeta'}{\zeta}(s) ds + \int_{\Gamma_6} (\widehat{\Phi}(s) + C) \frac{\zeta'}{\zeta}(s) ds \right] \\
 &= \lim_{j \rightarrow \infty} \frac{1}{2\pi i} \left[\left(\widehat{\Phi}(s) - C \right) \log \zeta(s) \Big|_2^{2+iT_j} + \left(\widehat{\Phi}(s) + C \right) \log \zeta(s) \Big|_{2-iT_j}^2 \right] \\
 &\quad - \frac{1}{2\pi i} \left[\int_{\Gamma_{5,6}} \widehat{\phi}(s) \log \zeta(s) ds \right] \\
 &= \frac{1}{2\pi i} \left[2C \log \zeta(2) - \int_{2-i\infty}^{2+i\infty} \widehat{\phi}(s) \log \zeta(s) ds \right],
 \end{aligned}$$

where $\Gamma_{5,6}$ denotes the contour Γ_5 followed by Γ_6 .

Considering the contours Γ_7 and Γ_8 , we use Lemma 4.3 and the Gaussian decay of $\widehat{\Phi}(s) \pm C$ from Lemma 4.6 to conclude that

$$\begin{aligned}
 \lim_{j \rightarrow \infty} (I_7 + I_8) &= \lim_{j \rightarrow \infty} \frac{1}{2\pi i} \left[\int_{\Gamma_7} (\widehat{\Phi}(s) - C) \frac{\zeta'}{\zeta}(s) ds + \int_{\Gamma_8} (\widehat{\Phi}(s) + C) \frac{\zeta'}{\zeta}(s) ds \right] \\
 &= 0.
 \end{aligned}$$

Considering I_9 and I_{10} we have

$$\begin{aligned}
 \lim_{j \rightarrow \infty} (I_9 + I_{10}) &= \lim_{j \rightarrow \infty} \frac{1}{2\pi i} \left[\int_{\Gamma_9} (\widehat{\Phi}(s) - C) \frac{\zeta'}{\zeta}(s) ds + \int_{\Gamma_{10}} (\widehat{\Phi}(s) + C) \frac{\zeta'}{\zeta}(s) ds \right] \\
 &= \lim_{j \rightarrow \infty} \frac{1}{2\pi i} \left[\left(\widehat{\Phi}(s) - C \right) \log(-\zeta(s)) \Big|_{-1+iT_j}^{1/4} \right. \\
 &\quad \left. + \left(\widehat{\Phi}(s) + C \right) \log(-\zeta(s)) \Big|_{1/4}^{-1-iT_j} \right] \\
 &\quad - \frac{1}{2\pi i} \left[\int_{\Gamma_9} \widehat{\phi}(s) \log(-\zeta(s)) ds + \int_{\Gamma_{10}} \widehat{\phi}(s) \log(-\zeta(s)) ds \right] \\
 &= -\frac{1}{2\pi i} \left[\int_{\Gamma_9, \Gamma_{10}} \widehat{\phi}(s) \log(-\zeta(s)) ds + 2C \log(-\zeta(1/4)) \right],
 \end{aligned}$$

where the contour of integration is Γ_9 followed by Γ_{10} . Convergence of this integral is due to Lemma 4.5 and the zero free region of $\zeta(s)$ with $|s+1| \leq \frac{5}{4}$ and $\Re s \geq -1$.

For I_{11} and I_{12} we have

$$\begin{aligned}
 I_{11} + I_{12} &= \frac{1}{2\pi i} \left[\int_{\Gamma_{11}} (\widehat{\Phi}(s) - C) \frac{\zeta'}{\zeta}(s) ds + \int_{\Gamma_{12}} (\widehat{\Phi}(s) + C) \frac{\zeta'}{\zeta}(s) ds \right] \\
 &= \frac{1}{2\pi i} \left[\left(\widehat{\Phi}(s) - C \right) \log(-\zeta(s)) \Big|_{1/4}^{1-\epsilon} + \left(\widehat{\Phi}(s) + C \right) \log(-\zeta(s)) \Big|_{1-\epsilon}^{1/4} \right] \\
 &\quad - \frac{1}{2\pi i} \left[\int_{\Gamma_{11}} \widehat{\phi}(s) \log(-\zeta(s)) ds + \int_{\Gamma_{12}} \widehat{\phi}(s) \log(-\zeta(s)) ds \right] \\
 &= \frac{1}{2\pi i} [2C \log(-\zeta(1/4)) - 2C \log(-\zeta(1-\epsilon))].
 \end{aligned}$$

For I_1 and I_2 we find

$$\begin{aligned}
 I_1 + I_2 &= \frac{1}{2\pi i} \left[\int_{\Gamma_1} (\widehat{\Phi}(s) - C) \frac{\zeta'}{\zeta}(s) ds + \int_{\Gamma_2} (\widehat{\Phi}(s) + C) \frac{\zeta'}{\zeta}(s) ds \right] \\
 &= \frac{1}{2\pi i} \left[\oint \widehat{\Phi}(s) \frac{\zeta'(s)}{\zeta(s)} ds - C \int_{\Gamma_1} \frac{\zeta'}{\zeta}(s) ds + C \int_{\Gamma_2} \frac{\zeta'}{\zeta}(s) ds \right] \\
 &= \widehat{\Phi}(1) - \frac{C}{2\pi i} \left[\int_{\Gamma_1} \frac{\zeta'}{\zeta}(s) ds - \int_{\Gamma_2} \frac{\zeta'}{\zeta}(s) ds \right]
 \end{aligned}$$

by Cauchy's Theorem since the residue of $\frac{\zeta'}{\zeta}(s)$ at $s = 1$ is -1 .

Finally, for I_3 and I_4 we get

$$\begin{aligned}
 I_3 + I_4 &= \frac{1}{2\pi i} \left[\int_{\Gamma_3} (\widehat{\Phi}(s) - C) \frac{\zeta'}{\zeta}(s) ds + \int_{\Gamma_4} (\widehat{\Phi}(s) + C) \frac{\zeta'}{\zeta}(s) ds \right] \\
 &= \frac{1}{2\pi i} \left[\left(\widehat{\Phi}(s) - C \right) \log \zeta(s) \Big|_{1+\epsilon}^2 + \left(\widehat{\Phi}(s) + C \right) \log \zeta(s) \Big|_2^{1+\epsilon} \right] \\
 &\quad - \frac{1}{2\pi i} \left[\int_{\Gamma_3} \widehat{\phi}(s) \log \zeta(s) ds + \int_{\Gamma_4} \widehat{\phi}(s) \log \zeta(s) ds \right] \\
 &= \frac{1}{2\pi i} [2C \log \zeta(1+\epsilon) - 2C \log \zeta(2)].
 \end{aligned}$$

Now by Cauchy's Theorem and exploiting the fact that the non-trivial zeros of ζ occur in complex conjugate pairs, $\lim_{j \rightarrow \infty} \sum_{k=1}^{12} I_k = \sum_{\rho} \Re \widehat{\Phi}(\rho)$ so we have

$$\begin{aligned} \sum_{\rho} \Re \widehat{\Phi}(\rho) &= \widehat{\Phi}(1) - \frac{1}{2\pi i} \left[\int_{2-i\infty}^{2+i\infty} \widehat{\phi}(s) \log \zeta(s) ds + \int_{\Gamma_9, \Gamma_{10}} \widehat{\phi}(s) \log(-\zeta(s)) ds \right] \\ &\quad + \frac{C}{\pi i} [\log \zeta(1+\epsilon) - \log(-\zeta(1-\epsilon))] \\ &\quad - \frac{C}{2\pi i} \left[\int_{\Gamma_1} \frac{\zeta'(s)}{\zeta(s)} ds - \int_{\Gamma_2} \frac{\zeta'(s)}{\zeta(s)} ds \right]. \end{aligned}$$

Now the result follows from taking the limit as $\epsilon \rightarrow 0^+$ by Lemmas 4.2 and 4.1 and then straightening the line of integration of the second integral to $\Re s = -1$. This introduces a contribution of $\log(-\zeta(0)) = -\log 2$ from the pole of $\widehat{\phi}(s)$ at $s = 0$ with residue 1. \square

Again, if we take $\widehat{\phi}(s) = \frac{x^s}{s}$, then $\widehat{\Phi}(s) = \text{Ei}(\log s)$, where Ei is the exponential integral and we recover Riemann's explicit formula

$$\pi^*(x) = \text{Ei}(\log x) - \sum_{\rho} \text{Ei}(\rho \log x) - \log 2 + \int_{-1-i\infty}^{-1+i\infty} \log(-\zeta(s)) x^s \frac{ds}{s}.$$

We truncate the sum over zeros so we need a rigorous bound for the error that this introduces. We derive such a bound in Appendix A.

The computation of $\pi(x)$ now reduces to

- enumerating the prime powers near x ,
- computing $\phi(t)$ at these prime powers,
- locating the non-trivial zeros of ζ to sufficient accuracy and
- evaluating $\widehat{\Phi}$ at these zeros (and at 1).

5. THE PRIME SIEVE AND $\phi(p)$

To compute $\pi(10^{24})$ with the zeros at our disposal we need a sieve of width $\approx 6 \times 10^{15}$ centred at 10^{24} . We only will discuss locating the primes in that interval, the prime powers being a trivial task by comparison.

Two basic methods were considered, sieving (necessarily segmented) and a hybrid technique described by Galway [8]. The latter proceeds by first eliminating all y -smooth numbers and then applying a base 2 Fermat primality test to the remainder. Given a list of the (few) numbers in our range which are composite, y -rough and yet still pass the Fermat test, we are done. Our tests suggest that while an implementation of the Hybrid sieve would not be competitive at height 10^{24} , the crossover might not be far away.

Our implementation used Atkin and Bernstein's sieve based on binary quadratic forms [2] to enumerate the sieving primes ($\leq x^{1/2}$) which are then used in a segmented version of the sieve of Eratosthenes to delete composites in the target region.

For each sieve segment centred at x_0 , we output

$$\sum_p 1, \sum_p (x_0 - p) \text{ and } \sum_p (x_0 - p)^2.$$

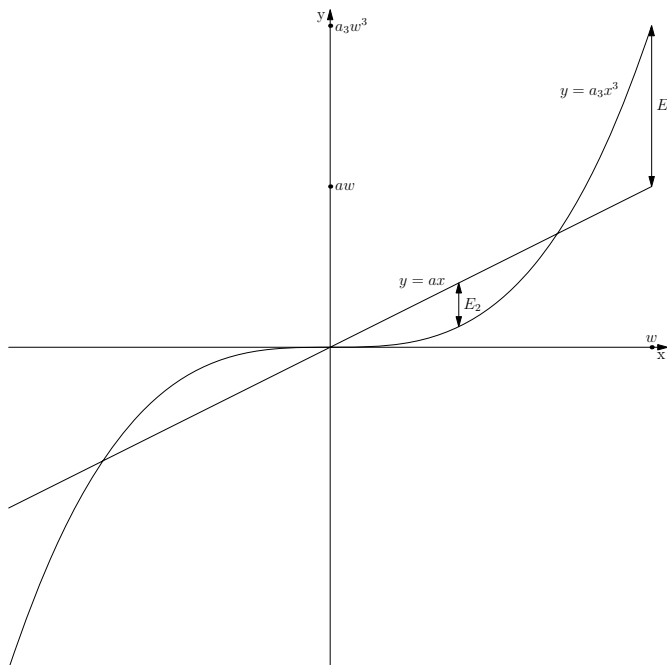


FIGURE 2. Approximating a cubic with a line (Lemma 5.1)

By restricting the sizes of the segments, we can ensure that the entire computation can be achieved using native 64 bit integer instructions, with the exception of the third sum which requires a 128 bit addition. However, this represents only a small performance penalty on modern CPUs. These three terms are then used to form an approximation to $\sum_p \phi(p)$ by the Taylor series. In fact, three terms are not enough to give us the required precision, so we exploit the following lemma to derive a linear approximation to the fourth (cubic) term as well.

Lemma 5.1. *If we approximate the real cubic $y = a_3x^3$ on the interval $x \in [-w, w]$ where $w > 0$ with the line $y = ax$ with $a = \frac{3a_3w^2}{4}$, then the magnitude of the error over the interval is $\leq \frac{|a_3|w^3}{4}$. What is more, in terms of minimising the worst case error, this line is the best choice of any quadratic.*

Proof. We refer to Figure 2. Without loss of generality, take $a_3 > 0$. Since both a_3x^3 and ax are odd, we consider only the interval $x \in [0, w]$. The error E_1 is simply $a_3w^3 - aw$, and E_2 is at its maximum where the slopes of the line and the cubic are equal. This happens at $x = \sqrt{\frac{a}{3a_3}}$ so $E_2 = \sqrt{\frac{a^3}{3a_3}} - \sqrt{\frac{a^3}{27a_3}}$. The worst case error follows from setting $E_1 = E_2$ and solving for a .

The maximum error occurs 4 times at $x \in \{\pm w, \pm\sqrt{\frac{a}{3a_3}}\}$. This means that any curve which improves on the line must be below the line at $x \in \{-w, \sqrt{\frac{a}{3a_3}}\}$ and above it at $x \in \{w, -\sqrt{\frac{a}{3a_3}}\}$. Thus, such a curve would have to cross the line at least 3 times, which is not possible for a quadratic. \square

6. COMPUTING $\widehat{\Phi}$

The following lemmas give us a means of computing $\Re\widehat{\Phi}(\rho)$.

Lemma 6.1. For $\Re s_0 \neq 0$ and $h \in \mathbb{R}$

$$\widehat{\phi}(s_0 + ih) = \widehat{\phi}(s_0) \exp(ih(s_0\lambda^2 + \log(x))) \frac{\exp\left(\frac{-\lambda^2 h^2}{2}\right)}{1 + \frac{ih}{s_0}}.$$

Proof. We start with

$$\widehat{\phi}(s_0 + ih) = \frac{\exp\left(\frac{\lambda^2(s_0 + ih)^2}{2}\right) x^{s_0 + ih}}{s_0 + ih}$$

and rearrange to get

$$\frac{\exp\left(\frac{\lambda^2 s_0^2}{2}\right) x^{s_0}}{s_0} \frac{\exp(ih(s_0\lambda^2 + \log(x))) \exp\left(\frac{-\lambda^2 h^2}{2}\right)}{1 + \frac{ih}{s_0}}.$$

□

Lemma 6.2. Let $N \in 2\mathbb{Z}_{>0}$, $\lambda, h > 0$ and $\lambda h < 1$. Then

$$\exp\left(\frac{-\lambda^2 h^2}{2}\right) = \sum_{n=0}^{\frac{N}{2}} \frac{(-1)^n}{n!} \left(\frac{\lambda^2 h^2}{2}\right)^n + E_A,$$

where

$$|E_A| \leq \frac{1}{\left(\frac{N}{2}\right)!} \left(\frac{\lambda^2 h^2}{2}\right)^{\frac{N}{2}}.$$

Proof. This function is entire, and the restriction on λh makes the terms alternating in sign and decreasing. □

Lemma 6.3. Let $N \in \mathbb{Z}_{>0}$, $R = \left|\frac{h}{s_0}\right|$ and $|h| < |s_0|$. Then

$$\left(1 + \frac{ih}{s_0}\right)^{-1} = \sum_{n=0}^N \left(\frac{-ih}{s_0}\right)^n + E_B$$

with

$$|E_B| \leq \frac{R^N}{1 - R}.$$

Proof. This function is analytic on the open disk $|h| < |s_0|$, and the missing terms form a geometric series. □

We can now fix some $N \in 2\mathbb{Z}_{>0}$ and multiply these two (degree N) polynomials to yield a single (degree $2N$) polynomial in h which we can integrate against $\exp(ih(\lambda^2 + \log(x)))$ analytically.

We now start at $\widehat{\Phi}\left(\frac{1}{2}\right)$ and move up the $\frac{1}{2}$ line in small steps. We take the contribution from the highest-used ρ to be zero and bound the error this approximation introduces.

7. THE COMPUTATION

To obtain the $\mathcal{O}(x^{1/2+\epsilon})$ time complexity of Lagarias and Odlyzko's algorithm, we should choose the free parameter λ to equate the run times of the sum over zeros and the sieving elements of the computation. In fact, we biased the run time towards computing zeros, both to confirm that the RH holds to a height sufficient for this computation and since this data may have application to future research.¹ We isolated all the zeros of ζ to a height of 30,610,046,000 (103,800,788,359 zeros). The technique used to locate these zeros is described in [15] but is in essence a ζ -specific, windowed version of Booker's algorithm from [4].

We set $\lambda = 6273445730170391 \times 2^{-84}$ (note that this is exactly representable in an IEEE 754 double precision floating point). We used the first 69,778,732,700 zeros to compute the sum (those to height 20,950,046,000) which in turn dictated that we sieve a region of width about 6×10^{15} . As a consequence, the truncation error from summing over the zeros and from the sieve were together < 0.989 .

With this choice of λ , we have $\left| \widehat{\Phi}\left(\frac{1}{2}\right) \right| < 3 \times 10^{13}$, so we need our zeros to be located to an absolute accuracy of at least 25 decimal places.² Thus, we are forced to use multiple precision arithmetic, despite the performance penalty this implies (up to a factor of 100 compared with the hardware floating point).

As discussed earlier, we use interval arithmetic to manage the accumulation of rounding errors during the computation, and to this end we have extended Revol and Rouillier's MPFI package [16] in the obvious way to handle complex arithmetic. Adopting interval arithmetic incurs another performance penalty (a factor of about 3 or 4 this time).

The sieving (entirely in integer arithmetic) was performed on 352,800 segments, each of width 2^{34} as dictated by memory constraints, further sub-divided to control the error in approximating ϕ by the Taylor series. The actual computation of this Taylor approximation again requires multiple precision interval arithmetic.

The sum over zeros and the prime sieve all parallelise trivially, and we used the University of Bristol Bluecrystal Phase II cluster to perform all the computations, consuming approximately 63,000 CPU hours. In a personal communication Tomás Oliveira e Silva indicated that computing $\pi(10^{23})$ using the combinatorial method required about a month on a single computer. Assuming run time asymptotic to $\mathcal{O}(x^{2/3})$ and $\mathcal{O}(x^{1/2})$ for the combinatorial and analytic algorithms respectively, the crossover at which this implementation of the analytic algorithm would start to beat the combinatorial method would be in the region of $x = 4 \cdot 10^{31}$.

The result of the computation, after adding in the various error terms, was an interval straddling a single integer, so we have

Theorem 7.1.

$$\pi(10^{24}) = 18,435,599,767,349,200,867,866.$$

We note that this agrees with the conditional result of Bütke, Franke, Jost and Kleinjung.

¹To this end, Jonathan Bober has made about the first 36 billion zeros available at [3].

²Our zeros are located to an absolute accuracy of $\pm 2^{-102}$, which more than suffices.

APPENDIX A. TRUNCATING THE SUM OVER ZEROS

We require a rigorous bound for the error introduced by truncating the sum over zeros in Theorem 4.7. We proceed as follows.

For $t > 0$, t not the imaginary part of a zero of ζ , define $N(t)$ to be the number of zeros of $\zeta(s)$ in the critical strip with $\Im s \in [0, t]$.

Lemma A.1. *Let $t \geq 2$. Then*

$$\left| N(t) - \frac{t}{2\pi} \log \left(\frac{t}{2\pi e} \right) - \frac{7}{8} \right| < 0.137 \log(t) + 0.443 \log \log(t) + 1.588.$$

Proof. See [17], Theorem 19. □

Lemma A.2. *For $x > 1$, $T, \lambda > 0$ and $\sigma \in [0, 1]$ define*

$$B(\sigma, T) := \exp \left(\frac{\lambda^2(1-T^2)}{2} \right) \left[\frac{x^\sigma}{T \log x} + \frac{1}{\lambda^2 T^2 x} \right].$$

Then

$$\left| \Re \widehat{\Phi}(\sigma + iT) \right| \leq B(\sigma, T).$$

Proof. We integrate along the contour running vertically down from $-1 + i\infty$ to $-1 + iT$, then right to $\sigma + iT$. For the horizontal contour we have

$$\begin{aligned} \left| \int_{-1}^{\sigma} \frac{\exp \left(\frac{\lambda^2(u+iT)^2}{2} \right)}{u+iT} x^{u+iT} du \right| &\leq \frac{\exp \left(\frac{\lambda^2(1-T^2)}{2} \right)}{T} \int_{-1}^{\sigma} x^u du \\ &< \frac{\exp \left(\frac{\lambda^2(1-T^2)}{2} \right)}{T \log x} x^\sigma. \end{aligned}$$

For the vertical contour we have

$$\begin{aligned} \left| \int_{\infty}^T \frac{\exp \left(\frac{\lambda^2(-1+it)^2}{2} \right)}{-1+it} x^{-1+it} dt \right| &\leq x^{-1} \exp \left(\frac{\lambda^2}{2} \right) \int_T^{\infty} \frac{\exp \left(\frac{-\lambda^2 t^2}{2} \right)}{t} dt \\ &< \frac{\exp \left(\frac{\lambda^2}{2} \right)}{x T^2} \int_T^{\infty} t \exp \left(\frac{-\lambda^2 t^2}{2} \right) dt \\ &= \frac{\exp \left(\frac{\lambda^2(1-T^2)}{2} \right)}{\lambda^2 T^2 x}. \end{aligned} \quad \square$$

Lemma A.3. *Let $T > 0$, $\sigma \in [0, 1]$ and α_T be such that $t^{\alpha_T} \geq N(t)$ for all $t \geq T$. Then*

$$\sum_{\Im \rho \geq T} B(\sigma, \Im \rho) \leq \exp \left(\frac{\lambda^2(1-T^2)}{2} \right) \left[\frac{x^\sigma}{T \log x} + \frac{1}{\lambda^2 T^2 x} \right] \left[\frac{\lambda^2 T^2 + 2}{\lambda^2 T^{2-\alpha_T}} - N(T) \right].$$

Proof. Referring to Lemma A.2 and by writing $k_\sigma := \exp \left(\frac{\lambda^2}{2} \right) \left[\frac{x^\sigma}{T \log x} + \frac{1}{\lambda^2 T^2 x} \right]$, we can majorise the sum with the Stieltjes integral

$$\int_T^{\infty} k_\sigma \exp \left(\frac{-\lambda^2 t^2}{2} \right) dN(t).$$

We now integrate by parts and majorise $N(t)$ with t^{α_T} to obtain

$$\begin{aligned} \sum_{\Im \rho > T} B(\sigma, \Im \rho) &\leq -k_\sigma \exp\left(\frac{-\lambda^2 T^2}{2}\right) N(T) - \frac{k_\sigma}{T^{2-\alpha_T}} \int_T^\infty \lambda^2 t^3 \exp\left(\frac{-\lambda^2 t^2}{2}\right) dt \\ &= k_\sigma \left[\frac{\lambda^2 T^2 + 2}{\lambda^2 T^{2-\alpha_T}} \exp\left(\frac{-\lambda^2 T^2}{2}\right) - \exp\left(\frac{-\lambda^2 T^2}{2}\right) N(T) \right]. \quad \square \end{aligned}$$

We note that the α_T referred to above can be computed using Lemma A.1.

We now consider the error introduced by truncating our sum over the zeros of ζ . Let T_1 be the height below which we find and use all the zeros, and T_2 the height to which we know the Riemann Hypothesis holds.

Lemma A.4. *Let E_1 be the real part of the error introduced by ignoring the zeros with imaginary part of absolute value $\in [T_1, T_2]$ (whose real parts are all known to be $\frac{1}{2}$). Then*

$$|E_1| \leq 2 \exp\left(\frac{\lambda^2(1 - T_1^2)}{2}\right) \left[\frac{\sqrt{x}}{T_1 \log x} + \frac{1}{\lambda^2 T_1^2 x} \right] \left[\frac{\lambda^2 T_1^2 + 2}{\lambda^2 T_1^{2-\alpha_{T_1}}} - N(T_1) \right].$$

Proof. We apply Lemma A.3 with $\sigma = \frac{1}{2}$ and introduce a factor of 2 for the zeros with negative imaginary part. \square

We note that this bound includes all the zeros with imaginary part $> T_2$, but their contribution will be negligible.

Lemma A.5. *Let E_2 be the real part of the error introduced by omitting the zeros with imaginary part $\notin [-T_2, T_2]$ from the main sum (which do not necessarily have real part $= \frac{1}{2}$). Then*

$$|E_2| \leq \exp\left(\frac{\lambda^2(1 - T_2^2)}{2}\right) \left[\frac{x+1}{T_2 \log x} + \frac{2}{\lambda^2 T_2^2 x} \right] \left[\frac{\lambda^2 T_2^2 + 2}{\lambda^2 T_2^{2-\alpha_{T_2}}} - N(T_2) \right].$$

Proof. We pair each ρ with $1 - \bar{\rho}$ and take the worst case, which is when one of the zeros has real part very close to 1. The result then follows from Lemma A.3. \square

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