Math 229: Introduction to Analytic Number Theory

The contour integral formula for $\psi(x)$

We now have several examples of Dirichlet series, that is, series of the form[1]

$$F(s) = \sum_{n=1}^{\infty} a_n n^{-s} \tag{1}$$

from which we want to extract information about the growth of $\sum_{n<x} a_n$ as $x\to\infty$. The key to this is a contour integral. We regard $F(s)$ as a function of a *complex* variable $s = \sigma + it$. For real $y > 0$ we have seen already that $|y^{-s}| = y^{-\sigma}$. Thus if the sum (1) converges absolutely[2] for some real σ_0, then it converges uniformly and absolutely to an analytic function on the half-plane $\mathrm{Re}(s) \geq \sigma_0$; and if the sum converges absolutely for all real $s > \sigma_0$, then it converges absolutely to an analytic function on the half-plane $\mathrm{Re}(s) > \sigma_0$. Now for $y > 0$ and $c > 0$ we have

$$\frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} y^s \frac{ds}{s} = \begin{cases} 1, & \text{if } y > 1; \\ \frac{1}{2}, & \text{if } y = 1; \\ 0, & \text{if } y < 1, \end{cases} \tag{2}$$

in the following sense: the contour of integration is the vertical line $\mathrm{Re}(s) = c$, and since the integral is then not absolutely convergent it is regarded as a principal value:

$$\int_{c-i\infty}^{c+i\infty} f(s)\, ds := \lim_{T\to\infty} \int_{c-iT}^{c+iT} f(s)\, ds.$$

Thus interpreted, (2) is an easy exercise in contour integration for $y \neq 1$, and an elementary manipulation of $\log s$ for $y = 1$. So we expect that if (1) converges absolutely in $\mathrm{Re}(s) > \sigma_0$ then

$$\sum_{n<x} a_n = \frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} x^s F(s) \frac{ds}{s} \tag{3}$$

for any $c > \sigma_0$, using the principal value of the integral and adding $a_x/2$ to the sum if x happens to be an integer. But getting from (1) and (2) to (3) involves interchanging an infinite sum with a conditionally convergent integral, which is not in general legitimate. Thus we replace $\int_{c-i\infty}^{c+i\infty}$ by $\int_{c-iT}^{c+iT}$, which legitimizes the manipulation but introduces an error term into (2). We estimate this error term as follows:

Lemma. *For $y, c, T > 0$ we have*

$$\frac{1}{2\pi i}\int_{c-iT}^{c+iT} y^s \frac{ds}{s} = \begin{cases} 1 + O(y^c \min(1, \frac{1}{T|\log y|})), & \textit{if } y \geq 1; \\ O(y^c \min(1, \frac{1}{T|\log y|})), & \textit{if } y \leq 1, \end{cases} \tag{4}$$

[1] As noted in [Serre 1973, Ch.6 §2], everything works just as well with "Dirichlet series" $\sum_{k=0}^{\infty} a_k n_k^{-s}$, where n_k are positive reals such that $n_k\to\infty$ as $k\to\infty$. In that more general setting we would seek to estimate $\sum_{n_k<x} a_k$ as $x\to\infty$.

[2] We shall see later that the same results hold if absolute convergence is replaced by conditional convergence throughout. For example, for every nonprincipal character χ the series for $L(s,\chi)$ converges uniformly in the half-plane $\mathrm{Re}(s) > \sigma_0$ for each positive σ_0.

the implied O-constant being effective and uniform in y, c, T.

(In fact the error's magnitude is less than both y^c and $y^c/\pi T\,|\log y|$. Of course if y *equals* 1 then the error term is regarded as $O(1)$ and is valid for both approximations $0, 1$ to the integral.)

Proof: Complete the contour of integration to a rectangle extending to real part $-M$ if $y \geq 1$ or $+M$ if $y \leq 1$. The resulting contour integral is 1 or 0 respectively by the residue theorem. We may let $M \rightarrow \infty$ and bound the magnitude of each horizontal integral by $(2\pi T)^{-1} \int_0^\infty y^{c \pm r} dr$; this gives the estimate $y^c/(\pi T\,|\log y|)$. Using a circular arc centered at the origin instead of a rectangle yields the same residue with a remainder of absolute value $< y^c$. $\square$

This Lemma will let us approximate $\sum_{n<x} a_n$ by $(2\pi i)^{-1} \int_{c-iT}^{c+iT} x^s F(s)\, ds/s$. We shall eventually choose some T and exploit the analytic continuation of F to shift the contour of integration past the region of absolute convergence to obtain nontrivial estimates.

Which F should we choose? Consider for instance $\zeta(s)$. We have in effect seen already that if we take $F(s) = \log \zeta(s)$ then the sum of the resulting a_n over $n < x$ closely approximates $\pi(x)$. Unfortunately, while $\zeta(s)$ continues meromorphically to $\sigma \leq 1$, its logarithm does not: it has essential logarithmic singularities at the pole $s = 1$ and at zeros of $\zeta(s)$ to be described later. So we use the *logarithmic derivative* of $\zeta(s)$ instead, which at each pole or zero of ζ has a simple pole with a known residue and thus a predictable effect on our contour integral.

What are the coefficients a_n for this logarithmic derivative? It is convenient to use not ζ'/ζ but $-\zeta'/\zeta$, which has positive coefficients. Using the Euler product we find

$$-\frac{\zeta'(s)}{\zeta(s)} = \sum_p \frac{d}{ds} \log(1 - p^{-s}) = \sum_p \log p \frac{p^{-s}}{1 - p^{-s}} = \sum_p \log p \sum_{k=1}^{\infty} p^{-ks}.$$

That is,

$$-\frac{\zeta'}{\zeta}(s) = \sum_{n=1}^{\infty} \Lambda(n) n^{-s}.$$

So the coefficient of n^{-s} is none other than the von Mangoldt function which arose in the factorization of $x!$. Hence our contour integral

$$\frac{1}{2\pi i} \int_{c-iT}^{c+iT} -\frac{\zeta'}{\zeta}(s)\, x^s \frac{ds}{s} \quad (c > 1)$$

approximates $\psi(x)$. The error can be estimated by our Lemma (4): since $|\Lambda(n)| \leq \log n$, the error is of order at most

$$\sum_{n=1}^{\infty} (x/n)^c \log n \cdot \min(1, \frac{1}{T\,|\log(x/n)|})$$

which is $O(T^{-1} x^c (\log^2 x + \frac{1}{c-1}))$ provided $1 < T < x$. (See the Exercises below.)

Now the factor x^c appearing in the error estimate exceeds x for any $c > 1$. To ensure that $x^c \ll x$, we fix some $A > 0$ and take $c = 1 + (A/\log x)$; this also makes the term $1/(c-1)$ negligible compared with $\log^2 x$. We then find:

$$\psi(x) = \frac{1}{2\pi i}\int_{1+\frac{A}{\log x}-iT}^{1+\frac{A}{\log x}+iT} -\frac{\zeta'}{\zeta}(s)\, x^s \frac{ds}{s} + O_A\left(\frac{x\log^2 x}{T}\right). \tag{5}$$

Similarly for any Dirichlet character χ we obtain a formula for

$$\psi(x,\chi) := \sum_{n<x} \chi(n)\Lambda(n)$$

by replacing $\zeta(s)$ in (5) by $L(s,\chi)$.

To make use of this, we want to shift the line of integration to the left, where $|x^s|$ is smaller. As we do this, we shall encounter a pole of $\zeta(s)$ at $s = 1$ and zeros of $\zeta(s)$ (or $L(s,\chi)$) at other values of s, leading us to estimate $|\zeta'(s)/\zeta(s)|$ (or $|L'(s,\chi)/L(s,\chi)|$) for s on the resulting contour. **This is why we are interested in the analytic continuation of $\zeta(s)$ and of $L(s,\chi)$, and in their zeros.** We investigate these matters next.

Remarks

We can already surmise that $\psi(x)$ will be approximated by $x - \sum_\rho x^\rho/\rho$, the sum running over zeros ρ of $\zeta(s)$ counted with multiplicity, and thus that the Prime Number Theorem is tantamount to the nonvanishing of $\zeta(s)$ on $\mathrm{Re}(s) = 1$. The fact that $\zeta(1+it) \neq 0$ is also the key step in various "elementary" proofs of the Prime Number Theorem such as [Newman 1980] (see also [Zagier 1997]). Likewise for $L(1+it,\chi)$ and the asymptotic formula for $\pi(x, a \bmod q)$.

The formula for $\psi(x)$ as a contour integral can be viewed as an instance of the inverse Mellin transform. Suppose $F(s)$ is a generalized Dirichlet series $\sum_{k=0}^{\infty} a_k n_k^{-s}$, converging for $\mathrm{Re}(s) > \sigma_0$. Let $A(x) = \sum_{n_k<x} a_k$, and assume that $A(x) \to \infty$ as $x \to \infty$. In particular, $\sigma_0 \geq 0$. Now

$$F(s) = \int_0^\infty x^{-s} dA(x) = s\int_0^\infty x^{-s} A(x)\frac{dx}{x},$$

so $F(s)/s$ is the Mellin transform of $A(x)$ evaluated at $-s$. Thus we expect that

$$A(x) = \frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} x^s F(s)\frac{ds}{s}$$

for $c > \sigma_0$. Due to the discontinuities of $A(x)$ at $x = n_k$, this integral cannot converge absolutely, but its principal value does equal $A(x)$ at all $x \notin \{n_k\}$.

Exercises

1. Verify that the error

$$\sum_{n=1}^{\infty} (x/n)^c \log n \cdot \min(1, \frac{1}{T\,|\log(x/n)|})$$

in our approximation of $\psi(x)$ is $O(T^{-1}x^c(\log^2 x + \frac{1}{c-1}))$ provided $1 < T < x$. Explain why the bound need not hold if T is large compared to x.

2. Use (4) to show that nevertheless $\psi(x)$ is given by the principal value integral

$$\psi(x) = \lim_{T\to\infty} \frac{1}{2\pi i} \int_{c-iT}^{c+iT} -\frac{\zeta'}{\zeta}(s)\, x^s \frac{ds}{s} \tag{6}$$

for all $x, c > 1$ such that $x \notin \mathbf{Z}$. What is the right-hand side of (6) when $c > 1$ and x is a positive integer?

3. Show that $\sum_{n=1}^{\infty} \mu(n) n^{-s} = 1/\zeta(s)$, with μ being the Möbius function defined in the previous set of exercises. Deduce an integral formula for $\sum_{n<x} \mu(n)$ analogous to (6), and an approximate integral formula analogous to (5) but with error only $O(T^{-1} x \log x)$ instead of $O(T^{-1} x \log^2 x)$.

References

[Newman 1980] Newman, D.J.: Simple Analytic Proof of the Prime Number Theorem, *Amer. Math. Monthly* **87** (1980), 693–696.

[Serre 1973] Serre, J.-P.: *A Course in Arithmetic.* New York: Springer, 1973 (Graduate Texts in Mathematics **7**).

[Zagier 1997] Zagier, D.: Newman's Short Proof of the Prime Number Theorem, *Amer. Math. Monthly* **104** (1994), 705–708.