18.785: Analytic Number Theory, MIT, spring 2007 (K.S. Kedlaya)
von Mangoldt's formula

In this unit, we derive von Mangoldt's formula estimating $\psi(x) - x$ in terms of the critical zeroes of the Riemann zeta function. This finishes the derivation of a form of the prime number theorem with error bounds. It also serves as another good example of how to use contour integration to derive bounds on number-theoretic quantities; we will return to this strategy in the context of the work of Goldston-Pintz-Yıldırım.

1 The formula

First, let me recall the formula I want to prove. Again, ψ is the function

$$\psi(x) = \sum_{n<x} \Lambda(n) + \frac{1}{2}\Lambda(x),$$

where Λ is the von Mangoldt function (equaling $\log p$ if $n > 1$ is a power of the prime p, and zero otherwise).

Theorem 1 (von Mangoldt's formula)**.** *For $x \geq 2$ and $T > 0$,*

$$\psi(x) - x = -\sum_{\rho:|\operatorname{Im}(\rho)|<T} \frac{x^\rho}{\rho} - \frac{\zeta'(0)}{\zeta(0)} - \frac{1}{2}\log(1 - x^{-2}) + R(x,T)$$

with ρ running over the zeroes of $\zeta(s)$ in the region $\operatorname{Re}(s) \in [0,1]$, and

$$R(x,T) = O\left(\frac{x\log^2(xT)}{T} + (\log x)\min\left\{1, \frac{x}{T\langle x\rangle}\right\}\right).$$

Here $\langle x\rangle$ denotes the distance from x to the nearest prime power other than possibly x itself.

2 Truncating a Dirichlet series

The basic idea is due to Riemann; it is to apply the following lemma to the Dirichlet series

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

(We will deduce this from Lemma 3 later.)

Lemma 2. *For any $c > 0$,*

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

where the contour integral is taken along the line $\operatorname{Re}(s) = c$.

To pick out the terms with $n \leq x$, use the integral from Lemma 2 with $y = x/n$; this gives

$$\psi(x) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} -\frac{\zeta'(s)}{\zeta(s)} \frac{x^s}{s} \, ds.$$

What we want to do is shift the contour of integration to the left, to pick up the residues at the poles of the integrand. Remember that for f meromorphic, $\frac{1}{2\pi i}\frac{f'}{f}$ has a simple pole at each s which is a zero or pole of f, and the residue is the order of vanishing (positive for a zero, negative for a pole) of f at s. In particular, the integrand we are looking at has only simple poles: the only pole of x^s/s is at $s = 0$, which is not a zero or pole of ζ.

We now compute residues. The pole of ζ at $s = 1$ contributes x, and every zero ρ of ζ (counted with multiplicity) contributes $-x^\rho/\rho$. This includes the trivial zeroes, whose contributions add up to

$$\sum_{n=1}^{\infty} -\frac{x^{-2n}}{(-2n)} = -\frac{1}{2}\log(1 - x^{-2}).$$

The only pole of x^s/s is at $s = 0$, and it contributes $-\zeta'(0)/\zeta(0)$.

We thus pick up all of the main terms in von Mangoldt's formula by shifting from the straight contour $c - iT \to c + iT$ to the rectangular contour $c - iT \to -U - iT \to -U + iT \to c + iT$, then taking the limit as $U \to \infty$. (We do have to make sure that the new contour does not itself does not itself pass through any poles of the integrand!) To prove the formula, it thus suffices to prove that:

- the discrepancy between the integral $c - iT \to c + iT$ and the full vertical integral $c - i\infty \to c + i\infty$,
- the horizontal integrals $c \pm iT \to -\infty \pm iT$, and
- the limit as $U \to -\infty$ of the vertical integral $-U - iT \to -U + iT$

are all subsumed by the proposed bound on the error term $R(x, T)$.

3 Truncating the vertical integral

We first replace the infinite vertical integral in Lemma 2 with a finite integral, and estimate the error term.

Lemma 3. *For $c, y, T > 0$, put*

$$I(y, T) = \frac{1}{2\pi i} \int_{c-iT}^{c+iT} y^s \frac{ds}{s},$$

with the integral taken along the straight contour, and

$$\delta(y) = \begin{cases} 0 & 0 < y < 1 \\ \frac{1}{2} & y = 1 \\ 1 & y > 1. \end{cases}$$

Then

$$|I(y,T)-\delta(y)| < \begin{cases} y^c \min\{1, T^{-1}|\log y|^{-1}\} & y \neq 1 \\ cT^{-1} & y = 1. \end{cases}$$

Proof. I'll do the case $0 < y < 1$ to illustrate, and leave the others for you. Note that there are two separate inequalities to prove; we establish them using two different contours.

Since y^s/s has no poles in $\mathrm{Re}(s) > 0$, for any $d > 0$, we can write

$$\int_{c-iT}^{c+iT} y^s \frac{ds}{s} = \int_{c-iT}^{d-iT} y^s \frac{ds}{s} - \int_{c+iT}^{d+iT} y^s \frac{ds}{s} + \int_{d-iT}^{d+iT} y^s \frac{ds}{s},$$

in which each contour is straight. As $d \to \infty$, the integrand in the third integral converges uniformly to 0. We can thus write

$$\int_{c-iT}^{c+iT} y^s \frac{ds}{s} = \int_{c-iT}^{\infty-iT} y^s \frac{ds}{s} - \int_{c+iT}^{\infty+iT} y^s \frac{ds}{s}$$

and each of the two terms is dominated by

$$\frac{1}{T}\int_c^\infty y^t\,dt = y^c T^{-1}|\log y|^{-1}.$$

Since we must then divide by $2\pi > 2$, we get one of the claimed inequalities.

Now go back and replace the original straight contour with a minor arc of a circle centered at the origin. This arc has radius $R = \sqrt{c^2+T^2}$, and on the arc the integrand y^s/s is dominated by y^c/R because $y < 1$. Thus the integral is dominated by $\pi R(y^c/R)$, and dividing by 2π yields the other claimed inequality. □

We will use Lemma 3 to show that

$$\int_{c-i\infty}^{c+i\infty} -\frac{\zeta'(s)}{\zeta(s)}\frac{x^s}{s}\,ds - \int_{c-iT}^{c+iT} -\frac{\zeta'(s)}{\zeta(s)}\frac{x^s}{s}\,ds = O\left(\frac{x(\log x)^2}{T} + (\log x)\min\left\{1, \frac{x}{T\langle x\rangle}\right\}\right).$$

By the lemma (applied with $y = x/n$), the left side is dominated by

$$\sum_{n=1, n\neq x}^{\infty} \Lambda(n)\left(\frac{x}{n}\right)^c \min\{1, T^{-1}|\log(n/x)|^{-1}\} + cT^{-1}\Lambda(x).$$

We get to choose any convenient value of c; it keeps the notation simple to take $c = 1 + (\log x)^{-1}$. Note that then $x^c = ex = O(x)$.

To estimate the summand, it helps to distinguish between terms where $\log(n/x)$ is close to zero, and those where it is bounded away from zero. For the latter, the quantity $|\log(n/x)|^{-1}$ is bounded above; so the summands with, say, $|n/x - 1| \geq 1/4$, are dominated by

$$O\left(xT^{-1}\left(-\frac{\zeta'(c)}{\zeta(c)}\right)\right) = O(xT^{-1}\log x).$$

For the former, consider values n with $3/4 < n/x < 1$ (the values with $1 < n/x < 5/4$ are treated similarly, and $n/x = 1$ contributes $O(\log x)$). Let x' be the largest prime power strictly less than x; then the summands $x' < n < x$ all vanish. In particular, it is harmless to assume $x' > 3x/4$, since otherwise the summands we want to bound all vanish.

We now separately consider the summand $n = x'$, and all of the summands with $3/4 < n < x'$. The former contributes

$$O\left(\log(x)\min\left\{1, \frac{x}{T(x-x')}\right\}\right).$$

For each term of the latter form, we can write $n = x' - m$ with $0 < m < x/4$, and

$$\log\frac{x}{n} \geq -\log\left(1 - \frac{m}{x'}\right) \geq \frac{m}{x'},$$

so these terms contribute

$$O\left(xT^{-1}(\log x)^2\right).$$

4 Shifting the contour

It remains to rewrite the integral

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

by shifting the contour and picking up residues. The new contour will be the three sides of the rectangle joining $c - iT, -U - iT, -U + iT, U + iT$ in that order, for suitable T and U.

We should choose U to be large and positive, so as to keep the vertical segment away from the trivial zeroes of ζ. Since those occur at negative even integers, we may simply take U to be a large *odd* positive integer.

It is a bit trickier to pick T. Note that we were actually given a value of T in the hypotheses of the theorem, but that T might be very close to the imaginary part of a zero of ζ. However, there is no harm in shifting T by a bounded amount: the sum over zeroes may change by the presence or absence of $O(\log T)$ terms each of size $O(xT^{-1}\log T)$, but we are allowing the error term to be as big as $O(xT^{-1}\log^2 T)$.

We now need to know how far away we can make T from the nearest zero, given that we can only shift by a bounded amount. This requires a slightly more refined count of zeroes than the one we gave before; see exercises.

Lemma 4. *The number of zeroes of ζ with imaginary part in $[T, T+1]$ is $O(\log T)$.*

This means we can shift T so that the difference between it and the imaginary part of any zero of ζ is at least some constant times $(\log T)^{-1}$.

We will also need a truncated version of the product representation of ζ'/ζ; see exercises.

Lemma 5. *For $s = \sigma + it$ with $-1 \leq \sigma \leq 2$ and t not equal to the imaginary part of any zero of ζ,*

$$\frac{\zeta'(s)}{\zeta(s)} = \sum_{\rho: |t - \mathrm{Im}(\rho)| < 1} \frac{1}{s - \rho} + O(\log |t|),$$

where ρ runs over critical zeroes of ζ.

Putting these two lemmas together, we deduce that (after shifting T by a bounded amount) for s on the contour with $\mathrm{Re}(s) \in [-1, 2]$,

$$\frac{\zeta'(s)}{\zeta(s)} = O(\log^2 T).$$

Thus the integrals over the horizontal contours $c - iT \to -1 - iT$ and $-1 + iT \to c + iT$ are

$$O\left(\log^2 T \int_{-1}^{c} |x^s/s|\, ds\right) \leq O\left(\frac{x \log^2 T}{T \log x}\right),$$

which is subsumed by our proposed error bound.

It remains to bound the integrals over the rectangular contour $-1 - iT \to -U - iT \to -U + iT \to -1 + iT$. For this, we use the functional equation for ζ, in the form

$$\zeta(1 - s) = \pi^{1/2 - s} \frac{\Gamma(s/2)}{\Gamma((1 - s)/2)} \zeta(s).$$

Using a classical identity (one of Legendre's duplication formulas for Γ), we can rewrite this as

$$\zeta(1 - s) = 2^{1-s} \pi^{-s} \cos(\pi s/2) \Gamma(s) \zeta(s).$$

We want to bound the log derivative of the left side; it is equal to the sum of the log derivatives of the various factors on the right side. The first two factors give constants. The third gives a constant times $\tan(\pi s/2)$, which is bounded if we keep s at a bounded distance from any odd integer. The fourth gives $\Gamma'(s)/\Gamma(s)$, which we proved in a previous exercise is $O(\log |s|)$ as $|s| \to \infty$ if $\mathrm{Re}(s) \geq 1/2$. The fifth gives $\zeta'(s)/\zeta(s)$, which is bounded as $|s| \to \infty$ if $\mathrm{Re}(s) \geq 2$.

Putting it all together, we deduce that if s is kept at a bounded distance from any negative even integer, we have

$$\frac{\zeta'(s)}{\zeta(s)} = O(\log |s|) \qquad (|s| \to \infty, \mathrm{Re}(s) \leq -1).$$

Applying this along the remaining rectangular contour, we bound the horizontal contributions by

$$O\left(\int_1^\infty (\log s + \log T) x^{-s}/T\, ds\right) \leq O\left(\frac{1}{Tx \log^2 x} + \frac{\log T}{Tx \log x}\right),$$

which is subsumed by our error bound. We bound the vertical contribution in the limit as $U \to 0$ by

$$O\left(\frac{T \log U}{U x^U}\right),$$

which tends to zero. We are done!

Exercises

1. Prove that for $T > 0$,
$$\sum_\rho \frac{1}{1 + (T - \mathrm{Im}(\rho))^2} = O(\log T),$$
where ρ runs over nontrivial zeroes of ζ. (Hint: this should have been on the previous handout. Go back to the proof of the zero-free region for ζ.)

2. Deduce Lemma 4 from the previous exercise.

3. Prove Lemma 5. (Hint: use the product representation for $\zeta'(s)/\zeta(s)$ evaluated at $s = \sigma + it$, then at $2 + it$, and subtract the two; everything left but the sum over ρ should be $O(\log |t|)$. Then use exercise 1 to control the contribution from the zeroes with $|t - \mathrm{Im}(\rho)| \geq 1$.) This can be used to derive a precise asymptotic for the number of zeroes of ζ in the critical strip with imaginary part in $(0, T)$:
$$\frac{T}{2\pi} \log \frac{T}{2\pi} - \frac{T}{2\pi} + O(\log T);$$
but I won't do so here. (See Davenport §15.)

4. Check the remaining cases of Lemma 3. (You should do $y = 1$ by a direct calculation. In the case $y > 1$, you should shift contours in the opposite direction, picking up the pole at $s = 0$.)