Section 6, The Prime Number Theorem

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1 Introduction.

The prime number theorem is one of the highlights of analytic number theory.

2 Chebychev facts

The material in this section may be found in many places, including Hardy and Wright, Jameson, and Apostol. But I strongly recommend the very nice writeup by Normal Levinson, from the MAA journal from 1969.

The prime number counting functions are

$$\begin{aligned}
\pi(x) &= \sum_{p\leq x} 1 = \#\left\{p \leq x\right\} \\
\theta(x) &= \sum_{p\leq x} \log(p) \\
\psi(x) &= \sum_{n\leq x} \Lambda(n) \ .
\end{aligned}$$

Here, $\Lambda(n)$ is the von Mangoldt function

$$\Lambda(n) = \begin{cases} \log(p) & \text{if } n = p^k \text{ for some prime } p \\ 0 & \text{otherwise, there is more than one prime in } n. \end{cases}$$

These definitions apply for any x. Of course, $\pi(x)$ (and $\theta(x)$ and $\psi(x)$) is constant on the interval $n \leq x < n+1$, so it really is only the integer values of x that matter. Still, it is convenient to have $\pi(x)$ defined for every x. The formulas and manipulations are simpler. For example, we will soon have the formula $\theta(\sqrt{x})$, which would be more complicated to write if we had defined θ only for integer arguments.

Any one of the following statements is the *prime number theorem*: as $x \to \infty$,

$$\pi(x) = \frac{x}{\log(x)} + o\left(\frac{x}{\log(x)}\right) \tag{1}$$

$$\theta(x) = x + o(x) \tag{2}$$

$$\psi(x) = x + o(x) \ . \tag{3}$$

Before the prime number theorem was proved, Chebychev learned two important things. One is the relation between $\pi(x)$, $\theta(x)$ and $\psi(x)$. Any of the statements (1) (2) (3) implies the other two. The π form (1) seems most natural, but we prove it by first proving the ψ form (3) and then using the equivalence. Chebychev also proved that the prime number theorem is true "up to a constant". Specifically, he showed that there are constants C_1 and C_2 so that

$$C_1 x \leq \psi(x) \leq C_2 x \ . \tag{4}$$

His proof is famous for being clever. It uses facts about the prime factorization of $n!$ and *Stirling's formula*, which is an estimate of the size of $n!$.

We start by finding inequalities for the quantities π, θ, and ψ in terms of the others. A simple one is

$$\theta(x) \leq \psi(x) \ . \tag{5}$$

This is because $\Lambda(n) \geq 0$ for all n, and $\Lambda(p) = \log(p)$. Therefore, every term in the ψ sum is at least as big as the corresponding term in the θ sum. This may be said more formally using a modification of $\Lambda(n)$:

$$L(n) = \begin{cases} \log(p) & \text{if } n = p \ \text{ for some prime } p \\ 0 & \text{if } n \text{ is not prime.} \end{cases}$$

Clearly (this was the point before), $\Lambda(n) \geq L(n)$ for every n. Also

$$\theta(x) = \sum_{n \leq x} L(n) \ .$$

This proves (5).

On the other hand, $\psi(x)$ is not much larger than $\theta(x)$. The terms in the ψ sum not in the θ sum are powers of primes. We will see that powers of primes (powers higher than one) are more rare than primes themselves. We see this by writing a different expression for $\psi(x)$. The non-zero terms in the ψ sum are from primes p with $p^k \leq x$. Therefore, we may write

$$\psi(x) = \sum_{p \leq x} \left(\sum_{p^k \leq x} \log(p) \right) \ .$$

The sum over $p^k \leq x$ is a sum over integers $k = 1, 2, \ldots$, up to the last k with $p^k \leq x$. Now, the inequality $p^k \leq x$ is equivalent to $p \leq x^{\frac{1}{k}}$. Therefore

$$\psi(x) = \sum_{p \leq x} \log(p) + \sum_{p \leq \sqrt{x}} \log(p) + \cdots + \sum_{p \leq x^{\frac{1}{k}}} \log(p) + \cdots \ .$$

The largest k value corresponds to the largest power of the smallest prime that is $\leq x$. This is $2^k \leq x$, which is $k \leq \log_2(x)$. But we like to use only $\log_e$, so we take the log base e to get

$$2^k \leq x \iff k \log(2) \leq \log(x) \iff k \leq \frac{\log(x)}{\log(2)} \ .$$

Note also that

$$\sum_{p\leq\sqrt{x}} \log(p) = \theta(\sqrt{x}) \ , \text{ etc.}$$

Combining these facts gives another expression for ψ:

$$\psi(x) = \sum_{k\leq\frac{\log(x)}{\log(2)}} \theta\left(x^{\frac{1}{k}}\right) \ .$$

The first term on the right is $\theta(x)$, which is supposed to be almost as big as $\psi(x)$. The rest of the terms on the right are supposed to be smaller. These are

$$\theta\left(x^{\frac{1}{2}}\right) + \theta\left(x^{\frac{1}{3}}\right) + \cdots \ .$$

Now, $x^{\frac{1}{3}} < x^{\frac{1}{2}}$ and $\theta(x)$ is a monotone non-decreasing function of x. Therefore

$$\theta\left(x^{\frac{1}{2}}\right) \leq \theta\left(x^{\frac{1}{3}}\right) \leq \cdots \leq \theta\left(x^{\frac{1}{k}}\right) \ .$$

The number of terms is one less than

$$k \leq \frac{\log(x)}{\log(2)} \ .$$

Therefore,

$$\theta\left(x^{\frac{1}{2}}\right) + \theta\left(x^{\frac{1}{3}}\right) + \cdots + \theta\left(x^{\frac{1}{k}}\right) \leq \frac{\log(x)}{\log(2)}\theta\left(x^{\frac{1}{2}}\right) \ .$$

This gives the inequality

$$\psi(x) \leq \theta(x) + C\log(x)\theta\left(x^{\frac{1}{2}}\right) \ . \tag{6}$$

In view of the (Chebychev) inequality $\theta(x) \leq Cx$, this shows that

$$|\psi(x) - \theta(x)| \leq C\log(x)\sqrt{x} \ .$$

Also in view of another Chebychev inequality $\psi(x) > Cx$, this shows that the difference between ψ and θ is much smaller than either θ or ψ, so the two quantities are about the same size. In particular, this shows that the θ and ψ forms of the prime number theorem, (2) and (3), are equivalent.

The relationship between $\theta(x)$ and $\pi(x)$ is essentially $\theta(x) \sim \log(x)\pi(x)$. This is (informally, not rigorously)

$$\theta(x) = \sum_{p\leq x} \log(p) \sim \sum_{p\leq x} \log(x) = \log(x)\pi(x) \ . \tag{7}$$

This is because, if $\epsilon > 0$, then most primes $p \leq x$ ("most" in the sense of the percentage of p that satisfy this), $\log(p) \geq (1-\epsilon)\log(x)$. We used a similar reasoning earlier in the semester to replace $\log(y)$ with $\log(x)$ in the integral and show that

$$\mathrm{li}(x) = \int_2^x \frac{1}{\log(y)}\, dy \approx \frac{x}{\log(x)} \; .$$

To get the conclusion (7), we must know that "most" primes are not small. This is the same as knowing that primes do not become too rare as x gets large. The whole thing may seem circular, since this would be a consequence of the prime number theorem, which we are trying to prove.

Instead of the intuitive approach (which can work) of the previous paragraph, here is a method that is easier to use, if harder to understand. The method uses *Abel summation*, which is a version of integration by parts for sums. For the integration by parts formula, suppose $f(x) = F'(x)$ and $g(x) = G'(x)$. Then

$$\int_a^b F(x)g(x)\, dx = F(b)G(b) - F(a)G(a) - \int_a^b f(x)G(x)\, dx \; .$$

This may be derived from the fundamental theorem of calculus and the product rule for derivatives:

$$\begin{aligned} F(b)G(b) - F(a)G(a) &= \int_a^b \frac{d}{dx}\left(F(x)G(x)\right)\, dx \\ &= \int_a^b f(x)G(x)\, dx + \int_a^b F(x)g(x)\, dx \; . \end{aligned}$$

Corresponding to indefinite integrals we have partial sums

$$A_n = \sum_1^n a_k \quad , \qquad B_n = \sum_{k=1}^n b_k \; .$$

Corresponding to derivatives, we have differences

$$a_n = A_n - A_{n-1} \quad , \qquad b_n = B_n - B_{n-1} \; .$$

By convention, we take $A_0 = 0$ and $B_0 = 0$. Integration by parts is a consequence of the product rule for differentiation and the fundamental theorem of calculus. Corresponding to the fundamental theorem of calculus, we have the sum

$$A_n B_n = \sum_{k=1}^n \left[A_k B_k - A_{k-1} B_{k-1} \right] \; .$$

Corresponding to the product rule for differentiation, we have

$$\begin{aligned} A_k B_k - A_{k-1} B_{k-1} &= A_k B_k - A_k B_{k-1} + A_k B_{k-1} - A_{k-1} B_{k-1} \\ &= A_k (B_k - B_{k-1}) + (A_k - A_{k-1}) B_{k-1} \\ &= A_k b_k + a_k B_{k-1} \; . \end{aligned}$$

Therefore

$$A_n B_n = \sum_{k=1}^{n} A_k b_k + \sum_{k=1}^{n} a_k B_{k-1} \; .$$

We make this look like integration by parts by rearranging the terms:

$$\sum_{k=1}^{n} A_k b_k = A_n B_n - \sum_{k=1}^{n} a_k B_{k-1} \; . \tag{8}$$

This is a form of the Abel summation formula. Notice that this formula is a little less symmetric than the integration by parts formula. The indices are the same on the left of (8), it's $A_k b_k$, but the indices are off by one on the right, where it's $a_k B_{k-1}$. For this reason, a mathematician may re-derive or look up the Abel summation formula when he/she uses it, but few of us forget the integration by parts formula.

We find inequalities relating $\pi(x)$ to $\theta(x)$ by applying Abel summation to the sequence $A_n = \log(n)$. This means that we must calculate (see how similar differencing and differentiation are)

$$a_k = \log(k) - \log(k-1) = \frac{1}{k} + O(k^{-2}) \; .$$

To see this, use the Taylor series remainder formula

$$f(x-y) = f(x) - f'(x)y - \frac{1}{2}f''(\xi)y^2 \; ,$$

for some $\xi \in [x-y, x]$. Specifically, we have $f(x) = \log(x)$, $f'(x) = x^{-1}$ and $f''(x) = -x^{-2}$, and $x = k$, and $y = 1$. We take the other series to be

$$b_n = \begin{cases} 1 & \text{if } n \text{ is prime} \\ 0 & \text{otherwise.} \end{cases}$$

Therefore, $B_n = \pi(n)$. We apply the Abel summation formula (8), and use the fact that the definition of b turns the right side into a sum over primes

$$\theta(n) = \sum_{p \leq n} \log(p) = \log(n)\pi(n) - \sum_{1}^{n} \frac{1}{k}\pi(k) + \sum_{1}^{n} \pi(k) O(k^{-2}) \; . \tag{9}$$

If we can ignore the sums on the right, we get

$$\theta(n) \approx \log(n)\pi(n) \; .$$

It is "easy" to handle the error terms, which are the sums on the right of (9). Anyway, it will become easy to do this kind of thing once you've done it enough times. Suppose we accept the Chebychev inequality $\pi(x) \leq Cx/\log(x)$. The second sum on the right is (because $1/\log(k) \leq 1$ for $k > 4$)

$$\leq C \sum_{1}^{n} \pi(k) k^{-2} \leq C \sum_{1}^{n} \frac{1}{k \log(k)} \leq C \sum_{1}^{n} \frac{1}{k} \leq C \log(n) \; .$$

This is a smaller order of magnitude than the left side, which is order n. The larger error sum on the right of (9) is

$$\sum_1^n \frac{1}{k}\pi(k) \leq C\sum_1^n \frac{1}{\log(k)} \sim \int^x \frac{1}{\log(y)}\,dy \leq C\frac{x}{\log(x)} \ .$$

Once these steps are justified, they show that the first sum also is smaller than $\theta(x)$. Note that the integral has the lower limit left out. That's because it is to some extent arbitrary. It matters only that it is fixed (independent of x) and large enough so that $\log(y) \neq 0$ in the range of integration. It would work to take $y = 2$ as the lower limit. The difference between this and, say, $y = 3$ is a constant independent of x.

It remains to justify the integral approximation to the sum and to prove the bound on the integral. For the bound on the integral, note that if $y \geq \sqrt{x}$, then $\log(y) \geq \frac{1}{2}\log(x)$. We can break the integral into two parts

$$\int_2^x \frac{1}{\log(y)}\,dy = \int_2^{\sqrt{x}} \frac{1}{\log(y)}\,dy + \int_{\sqrt{x}}^x \frac{1}{\log(y)}\,dy \ .$$

For $y > 2$, $\log(y) > C > 0$ (because $\log(2) > 0$) so

$$\int_2^{\sqrt{x}} \frac{1}{\log(y)}\,dy \leq C\sqrt{x} \ .$$

In the second integral, the integrand satisfies

$$\frac{1}{\log(y)} \leq \frac{1}{\frac{1}{2}\log(x)} = \frac{2}{\log(x)} \ .$$

Therefore,

$$\int_{\sqrt{x}}^x \frac{1}{\log(y)}\,dy \leq \frac{2x}{\log(x)} \ .$$

We can combine these two estimates to get the bound we used above:

$$\int_2^x \frac{1}{\log(y)}\,dy \leq \frac{Cx}{\log(x)} \ .$$

Mathematicians who do this kind of analysis, either in analytic number theory or other areas, spend many of their waking hours constructing ad-hoc arguments like this. It's part of the donkey-work of theoretical mathematics.

We can justify bounding the sum by the integral in several ways. One way is to say

$$\frac{1}{\log(k)} \leq \int_{k-1}^k \frac{1}{\log(y)}\,dy$$

Then

$$\sum^x \frac{1}{\log(k)} \leq \int^x \frac{1}{\log(y)}\,dy \ .$$

You might want to think about where the sum and integral have to start. But since both go to infinity as $x \to \infty$, it's OK to be off by a constant that is independent of x.

The integral estimate is not "sharp" because we don't know the constant C. Our method for getting non-sharp bounds can be used to get sharper bounds. This is unnecessary here, but (some) mathematicians feel compelled to do it anyway. Using integration by parts, we find

$$\int^x \frac{1}{\log(y)}\, dy = \frac{x}{\log(x)} + C + \int^x \frac{1}{\log^2(y)}\, dy \ .$$

The value of C depends on the un-written lower limit. Our non-sharp estimate (the technique used to get it) leads to

$$\int^x \frac{1}{\log^2(y)}\, dy \leq \frac{Cx}{\log^2(x)} \ .$$

Therefore

$$\int^x \frac{1}{\log(y)}\, dy = \frac{x}{\log(x)} + O\!\left(\frac{x}{\log^2(x)}\right) \ .$$

Here, the error term with $\log^2(x)$ is smaller, as $x \to \infty$ than the main term with $\log(x)$. The sharp coefficient in the main term is $C = 1$.

We just showed how to learn about θ once you know about π. A variant on that method allows us to do the reverse, to learn about π from θ. For that, we take

$$A_n = \frac{1}{\log(n)} \ .$$

The first two derivatives are

$$A_n \xrightarrow{\frac{d}{dn}} \frac{-1}{n\log^2(n)} \xrightarrow{\frac{d}{dn}} \frac{1}{n^2\log^2(n)} + \frac{2}{n^2\log(n)^3} \ .$$

Therefore (mean value theorem with $\Delta n = 1$, and $n^{-2}\log(n)^{-3} = O(n^{-2})$), we have (Note that this is not sharp, the $\log(n)$ part was dropped because it isn't needed.)

$$a_n = \frac{-1}{n\log^2(n)} + O(n^{-2})$$

We take

$$b_n = \begin{cases} \log(p) & \text{if } n = p \text{ is prime} \\ 0 & \text{otherwise.} \end{cases}$$

The Abel summation formula, with these definitions, is

$$\begin{aligned}\sum_{p\leq n} 1 &= \sum_{k\leq n} \frac{1}{\log(k)}(\theta(k) - \theta(k-1)) \\ &= \frac{1}{\log(n)}\theta(n) + \sum_1^n \frac{\theta(k)}{k\log^2(k)} + \sum_1^n O\!\left(\frac{\theta(k)}{k^2}\right) \ .\end{aligned}$$

The left side, by design, is $\pi(x)$. If $\theta(x) \approx Cx$, then the first error term on the right is

$$\leq C \sum_{1}^{n} \frac{1}{\log^2(k)} \leq C \frac{x}{\log^2(x)}$$

This is smaller than the main term, which would be

$$\frac{\theta(n)}{\log(n)} \approx \frac{Cn}{\log(n)} \; .$$

The error term is smaller, but only by a log. Error estimates in the prime number theorem are famous for being weak in this way.

This may seem like a lot of material, but there is nothing particularly clever about it. Abel summation is a well known trick that you just try and hope for the best. It works in this instance because it is a way of showing that $\log(n) \approx \log(k)$ for most k in the range $[1, n]$. The differences $\log(k) - \log(k-1)$ are small, so the "boundary term" $A_n B_n$ is larger (just barely) than the "correction terms" that are the sums on the right side.

The upper and lower bounds on $\psi(x)$ are more clever. They rely on the observation of Chebychev that you can figure out which primes occur how many times in $N = n!$. Clearly, only primes $p \leq n$ can appear. Since $n!$ is much larger than n, we see that $N = n!$ is a large number that has no large prime factors.

In the version of Levinson, we define a version of $\log(n!)$ for general real argument x:

$$T(x) = \sum_{n \leq x} \log(n) \; .$$

If n is an integer, then $T(n) = \log(n!)$. Like $\psi(x)$ and $\pi(x)$, $T(x)$ is constant in the interval $n \leq x < n+1$. For integer n, Stirling's approximation (a derivation is an exercise) gives

$$T(n) = \log(n!) = n \log(n) - n + O(\log(n)) \; .$$

Is this true for general real argument x? The function $x \log(x) - x$ is an increasing function of x, but $T(x) = T(n)$ if $n \leq x < n+1$. If x is close to $n+1$, it might be that $x \log(x) - x$ is more than $O(\log(x))$ larger than $n \log(n) - n$. The worst case is $x = n+1$, so we calculate

$$\log((n+1)!) = (n+1)\log(n+1) - (n+1) + O(\log(n+1)) \; .$$

Some "routine" calculations (an exercise) show that this is $n \log(n) - n + O(\log(n))$. Therefore, we may write

$$T(x) = x \log(x) - x + O(\log(x)) \; . \tag{10}$$

Chebychev's trick, in the version of Levinson, is to express $T(x)$ in terms of ψ. This starts with an expression for $\log(n)$ in terms of Λ. If $n = p_1^{r_1} \cdots p_k^{r_k}$

(the prime factorization of n), then (explanation below)

$$\log(n) = r_1 \log(p_1) + \cdots + r_k \log(p_k) = \sum_{j|n} \Lambda(j) \ .$$

The notation $j|n$ means that the sum is over all divisors of n. If j is a divisor of n, then $\Lambda(j) = 0$ if j has more than one prime. Therefore, the only non-zero terms are from $j = p_i^m$, where p_i is one of the prime factors of n and $1 \leq m \leq r_i$. Each one of these gives a contribution of $\log(p_i)$, so there are r_i contributions of $\log(p_i)$. This may be re-written in the form

$$\log(n) = \sum_{jk=n} \Lambda(j) \ . \tag{11}$$

We can sum over $n \leq x$ to get

$$T(x) = \sum_{jk \leq x} \Lambda(j) \ .$$

The sum is over all integer pairs j, k with $jk \leq x$. This may be rewritten with the sum over j on the inside

$$T(x) = \sum_{k \leq x} \left(\sum_{j \leq \frac{x}{k}} \Lambda(j) \right)$$

$$T(x) = \sum_{k \leq x} \psi(x/k) \ . \tag{12}$$

This formula shows the convenience of defining $\psi(x)$ for non-integer x.

Now the cleverness starts. We apply (12) to $T(x/2)$ then subtract $2T(x/2)$ from $T(x)$. The result is

$$\begin{aligned} T(x) &= \psi(x) + \psi(x/2) + \psi(x/3) + \psi(x/4) + \psi(x/5) + \psi(x/6) + \cdots \\ T(x/2) &= \qquad\quad\ \psi(x/2) + \qquad\qquad\ \psi(x/4) + \qquad\qquad\ \psi(x/6) + \cdots \\ T(x) - 2T(x/2) &= \psi(x) - \psi(x/2) + \psi(x/3) - \psi(x/4) + \psi(x/5) - \psi(x/6) + \cdots \ . \end{aligned}$$

From Stirling's approximation (10), we calculate

$$T(x) - 2T(x/2) = x \log(x) - x - 2 \left[\frac{x}{2} \log(x/2) - \frac{x}{2} \right] + O(\log(x))$$

$$T(x) - 2T(x/2) = x \log(2) + O(\log(x)) \ .$$

Now, ψ is a non-decreasing function, so $\psi(x/2) - \psi(x/3) \geq 0$, and so on. Therefore,

$$T(x) - 2T(x/2) = \psi(x) - (\text{positive}) - (\text{positive}) - \cdots$$

$$T(x) - 2T(x/2) \leq \psi(x) \ .$$

This leads to Chebychev's lower bound for ψ, which is

$$\psi(x) \geq \log(2)x + O(\log(x)) \ . \tag{13}$$

We expect $\psi(x) = x + o(x)$, so we should note that the constant $\log(2)$ is positive (because $2 > 1$) but less than 1 (because $2 < e$). The actual value is $\log(2) = .693....$

The Chebychev upper bound keeps the first two terms on the right. Because ψ is increasing, we have $\psi(x/3) - \psi(x/4) \geq 0$, etc. Therefore

$$T(x) - 2T(x/2) = \psi(x) - \psi(x/2) + (\text{positive}) + (\text{positive}) - \cdots \ ,$$

so

$$\psi(x) - \psi(x/2) \leq \log(2)x + O(\log(x)) \ .$$

We want to use this to prove $\psi(x) \leq Cx + O(\log(x))$. It will be a proof by induction. The cases $x = 2, 3, 4$ are clear. So, suppose you know that $\psi(x/2) \leq (C/2)x + O(\log(x))$ and you want to use

$$\psi(x) \leq \log(2)x + (C/2)x + O(\log(x))$$

to prove $\psi(x) \leq Cx + O(\log(x))$. From the inequality, it seems that we might take C to satisfy

$$Cx = \log(2)x + (C/2)x \implies C = \log(2) + \tfrac{1}{2}C \implies C = 2\log(2) \ .$$

Indeed, if we know by induction that $\psi(x) \leq 2\log(2)x = O(\log(x))$, then we conclude that

$$\psi(x) \leq \log(x)x + \tfrac{1}{2}2\log(2)x + O(\log(x)) \ .$$

This proves the Chebychev upper bound

$$\psi(x) \leq 2\log(2)x + O(\log(x)) \ . \tag{14}$$

The constant is $2\log(2) = 1.386... > 1$, which is consistent with the prime number theorem.

3 Contour integral of ζ

We saw that if $\sigma > 0$,

$$\frac{1}{2\pi i}\int_{\sigma - i\infty}^{\sigma + i\infty} \frac{x^s}{sn^s}\, ds = \begin{cases} 1 & \text{if } n < x \\ 0 & \text{if } n > x \ . \end{cases}$$

We also have, for $\sigma > 1$,

$$-\frac{\zeta'(s)}{\zeta(s)} = \sum_1^\infty \Lambda(n) n^{-s} \ . \tag{15}$$

Therefore, it's natural to think that, for $\sigma > 1$,

$$\frac{-1}{2\pi i}\int_{\sigma-i\infty}^{\sigma+i\infty}\frac{x^s}{s}\frac{\zeta'(s)}{\zeta(s)}\,ds = \sum_{n<x}\Lambda(n) = \psi(x)\ . \tag{16}$$

Riemann's strategy was to move (deform) the contour to $\sigma < 1$. The integrand

$$\frac{x^s}{s}\frac{\zeta'(s)}{\zeta(s)}$$

has a simple pole at $s = 1$ with residue X. We saw that the residue of ζ'/ζ is -1. Therefore[1], the residue of the product is -1 multiplied by the value of x^s/s when $s = 1$, giving $-x$. The integrand also would have poles at values ρ where $\zeta(\rho) = 0$. (Zeros of ζ are called ρ.) Riemann believed – and modern mathematicians still believe – that there are no zeros with $\mathrm{Re}(\rho) > \frac{1}{2}$. This is the *Riemann hypothesis*, perhaps the most important unsolved problem in matheamtics today. If the Riemann hypothesis is true (and some other things), we should be able to move the contour in (16) to σ_0 with $\frac{1}{2} < \sigma_0 < 1$. So, take $\sigma_1 > 1$ and $\frac{1}{2} < \sigma_0 < 1$. Imagine a closed contour that goes "up" the σ_1 part to $+\infty$ (or very high), then to σ_0, then down the σ_0 contour to $-\infty$ (or very low), then back to σ_1. There should be only one pole inside that contour, with residue x, so (notice the overall minus sign)

$$\frac{-1}{2\pi i}\int_{\sigma_1-i\infty}^{\sigma_1+i\infty}\frac{x^s}{s}\frac{\zeta'(s)}{\zeta(s)}\,ds + \frac{-1}{2\pi i}\int_{\sigma_0-i\infty}^{\sigma_0+i\infty}\frac{x^s}{s}\frac{\zeta'(s)}{\zeta(s)}\,ds = x\ .$$

With (16), that gives

$$\psi(x) = x + \frac{-1}{2\pi i}\int_{\sigma_0-i\infty}^{\sigma_0+i\infty}\frac{x^s}{s}\frac{\zeta'(s)}{\zeta(s)}\,ds\ . \tag{17}$$

The integral over the σ_0 contour is supposed to be on the order of $x^{\sigma_0} = o(x)$ because it is

$$x^{\sigma_0}\int_{-\infty}^{\infty} e^{it\log(x)}\frac{\zeta'(\sigma_0+it)}{(\sigma_0+it)\zeta(\sigma_0+it)}\,idt\ .$$

Riemann then argued that the integral is the Fourier transform of the function

$$f(t) = \frac{\zeta'(\sigma_0+it)}{(\sigma_0+it)\zeta(\sigma_0+it)}$$

and this function goes to zero as $t \to \pm\infty$. What is now called the *Riemann Lebesgue lemma* is the statement that (under the right hypotheses) Fourier

[1] We saw that $\zeta(s) = \frac{1}{s-1} + h(s)$, with h analytic near $s = 1$. Therefore, $\zeta' s = \frac{-1}{(s-1)^2} + h'(s)$. Informally, we write $\zeta(s) \approx \frac{1}{s-1}$ and $\zeta'(s) \approx \frac{-1}{(s-1)^2}$. Then $\zeta'(s)/\zeta(s) \approx [-1/(s-1)^2][1/(s-1) = -1/(s-1)$. The power of complex analysis is that these calculations are legit; ζ'/ζ does have residue -1 at $s = 1$.

transforms go to zero, in this case, as $\log(x) \to \infty$. This (more or less) is how Riemann arrived at the statement

$$\psi(x) = x + o(x) \quad \text{as } x \to \infty ,$$

which is the prime number theorem.

Now we have to compare what was hoped for to what can be proven. A proof of the prime number theorem, one using the zeta function, has to learn more about the behavior of $\zeta(s)$ in and around the *critical strip*, which is $s = \sigma + it$ for $0 \le \sigma \le 1$. It also calls for workarounds for the facts about ζ that cannot, yet, be proven. The details will be rather "technical", which means that they will involve approximating integrals and sums simultaneously with enough accuracy to get $o(x)$ in the $\psi(x)$ error estimate. Instead of integrating over the whole σ_1 contour, we integrate in the range $|t| \le T$ and ask how the error depends on t. We choose $T \to \infty$ as $x \to \infty$ to remove this error. We also choose $\sigma_1 \downarrow 1$ as $x \to \infty$. There will be an error depending on x^{σ_1}. For example, we can make $x^{\sigma_1} = x\log(x)$ by with the appropriate choice of σ_1 as a function of x.

What can we prove about $\zeta(\sigma + it)$? Rather straightforward estimates of the Dirichlet series show that if $t > 1$, then

$$|\zeta(1 + it)| \le C \log(t) .$$

This applies also to ζ'. There is a clever (how did anyone think of this??) argument to show that there are no zeros on the line $\sigma = 1$. There is a *zero free region* in the critical strip that includes the line $\sigma = 1$. This small zero free region is enough to get started moving the contour into the critical strip. We learn about ζ on the line $\sigma = 0$ using the *Riemann functional equation*. It also gives bounds for $\zeta'(1 + it)/\zeta(1 + it)$ as $t \to \infty$.

4 Simple facts about $\zeta(1 + it)$

We need bounds on $\zeta(\sigma + it)$ for large t and σ near 1. These are used to estimate the contour integral the line $\sigma = 1$. We find the bounds directly from the Dirichlet sum of $n^{-s} = n^{-\sigma} e^{-it\log(n)}$. We would like to approximate the sum by an integral, but the approximation

$$n^{-s} \approx \int_n^{n+1} y^{-s}\, ds \tag{18}$$

is inaccurate if t is large and n is not large. Therefore, we split the Dirichlet series into a low n part where no approximation is possible and a large n part where the approximation applies. We choose N depending on t and write

$$\zeta(s) = \sum_{n=1}^{N-1} n^{-s} + \sum_{N}^{\infty} n^{-s} = D_1(s) + D_2(s) .$$

We will get a bound for $D_1(s)$ that goes to infinity as $N \to \infty$. Our bound on $D_2(s)$ goes to zero as $N \to \infty$, but only applies if N is above a certain value, depending on t. In the end, we choose N as a function of t to optimize (minimize) the sum of the two inequalities.

Start with the small n sum $D_1(s)$. The terms $e^{-it\log(n)}$ are unit length complex numbers that point in different directions. There is likely to be a lot of *cancellation* in the sum, as terms in different directions are added together. Cancellation means that the magnitude of the sum is much smaller than the sum of the magnitudes of the terms. We ignore that possibility and just sum the magnitudes of the terms

$$\begin{aligned}
|D_1(s)| &= \left| \sum_1^{N-1} n^{-\sigma} e^{-it\log(n)} \right| \\
&\leq \sum_1^{N-1} \left| n^{-\sigma} e^{-it\log(n)} \right| \\
D_1(s) &\leq \sum_1^{N-1} n^{-\sigma} \ .
\end{aligned}$$

For $\sigma = 1$ (the right edge of the *critical strip*), the result is

$$|D_1(1+it)| \leq C\log(N) \ .$$

This goes to infinity as $N \to \infty$, so we hope it is possible to let N go to infinity slowly.

The D_2 part is the part where the approximation (18) applies. The bound on D_2 would come from

$$\begin{aligned}
D_2(s) &= \sum_N^{\infty} n^{-s} \\
&= \int_N^{\infty} y^{-s}\, dy + (\text{error}) \\
&= \frac{1}{s-1} N^{-(s-1)} + (\text{error}) \\
|D_2(s)| &= \frac{1}{|\sigma - 1 + it|} N^{-(\sigma-1)} + (\text{error}) \ .
\end{aligned} \tag{19}$$

Ignoring the error term for a moment, calculating the integral explicitly captures cancellation in the D_2 sum. The bound is particularly simple when $\sigma = 1$. If $\sigma = 1 - \epsilon$ (a little smaller than 1, in the critical strip), then we have N^{ϵ}. This goes to infinity as $N \to \infty$, which is not what we want. We still can use the bound if $\epsilon \to 0$ as $t \to \infty$ or $N \to \infty$. Mathematical analysis, as done by working mathematicians, often turns into this kind of game.

How large must n be for the approximation (18) to be valid? It is based on

$$k^{-s} = \int_k^{k+1} x^{-s}\, dx + \int_k^{k+1} \left(k^{-s} - x^{-s} \right)\, dx \ .$$

The first term on the right leads to the integral in D_2. The second term is the error term, which we just want to bound. The Taylor series bound is

$$\left|k^{-s} - x^{-s}\right| \leq |k - x| \max_{k \leq y \leq x} \left|\frac{d}{dy} y^{-s}\right| \ .$$

We are not using the intermediate value theorem because these quantities are complex if $s = \sigma + it$ is complex, while the intermediate value theorem is for real functions of a real variable. If $y \geq k$, then (recall that $\left|y^{-it}\right| = \left|e^{-it\log(y)}\right| = 1$)

$$\begin{aligned}
\left|\frac{d}{dy} y^{-s}\right| &= \left|-sy^{-(s+1)}\right| \\
&\leq |s| \left|y^{-(\sigma+1)} y^{-it}\right| \\
&\leq |s| \left|y^{-(\sigma+1)}\right| \\
&\leq |s| \, k^{-(\sigma+1)} \ .
\end{aligned}$$

We can now add up all the (error) terms in (19). The result is

$$(\text{error}) \leq \sum_{N+1}^{\infty} |s| \, k^{-(\sigma+1)} \leq C \, |s| \, N^{-\sigma} \ .$$

If $|t| \geq 2$ (2 is arbitrary, but we're not interested in getting constants right here) and $\sigma \leq 2$ (we want to get close to the critical strip) then (using $\sqrt{2} < 2$ and $\sigma^2 \leq t^2$)

$$|s| = \left(\sigma^2 + t^2\right)^{\frac{1}{2}} \leq \left(2t^2\right)^{\frac{1}{2}} \leq 2\,|t| \ .$$

On the line $\sigma = 1$,the D_2 bound is

$$D_2(s) \leq C \left(1 + |t| \, N^{-1}\right) \ .$$

Then D_2 is bounded and $D_1 \leq C \log(|t|)$. Altogether,

$$|\zeta(1 + it)| \leq C \log(t) \ . \tag{20}$$

This shows that on the line $\sigma = 1$, the zeta function is almost bounded as $t \to \infty$, but not quite. You might wonder whether someone with more skill and patience with mathematical analysis could get rid of the logarithmic growth.

The contour integral in (17) has $\zeta(s)$ in the denominator. Therefore, we should know where $\zeta(s) = 0$. The Euler product representation for $\zeta(s)$ implies that $\zeta(s) \neq 0$ if $\sigma > 1$. But it leaves the possibility that $\zeta(\sigma + it) \to 0$ as $\sigma \downarrow 1$. This does not happen. The proof involves the fact that

$$3 + 4\cos(\theta) + \cos(2\theta) \geq 0 \ , \quad \text{for all real } \theta \ . \tag{21}$$

Here is a proof. Every cosine may be represented as

$$x = \cos(\theta) = \frac{z + \overline{z}}{2} = \frac{z + z^{-1}}{2}$$

for some complex z with $|z| = 1$ (take $z = e^{i\theta}$). Then

$$\cos(2\theta) = \frac{z^2 + z^{-2}}{2} = \frac{z^2 + 2 + z^{-2}}{2} - 1 = \frac{\left(z + z^{-1}\right)^2}{2} - 1 \; .$$

We calculate:

$$\begin{aligned} 3 + 4\cos(\theta) + \cos(2\theta) &= 3 + 4\frac{z + z^{-1}}{2} + \frac{\left(z + z^{-1}\right)^2}{2} - 1 \\ &= 2 + 4\frac{z + z^{-1}}{2} + 2\left(\frac{z + z^{-1}}{2}\right)^2 \\ &= 2\left(1 + 2x + x^2\right) \\ &= 2\left(1 + x\right)^2 \\ &\geq 0 \; . \end{aligned}$$

I don't know how Hadamard realized that this simple inequality could be used as it is about to be used. You will see that it is crucial that $4 > 3$.

Suppose $f(s)$ is a convergent Dirichlet series with non-negative coefficients:

$$f(s) = \sum_1^\infty a_n n^{-s} \; .$$

For $s = \sigma + it$, the real part of n^{-s} is

$$\mathrm{Re}\left(n^{-s}\right) = \mathrm{Re}\left(n^{-\sigma} n^{-it}\right) = n^{-\sigma}\mathrm{Re}\Big(e^{-it\log(n)}\Big) = n^{-\sigma}\cos(t\log(n)) \; .$$

If the a_n are real, then

$$\mathrm{Re}\left(f(\sigma + it)\right) = \sum_1^\infty a_n n^{-\sigma}\cos(t\log(n)) \; .$$

We apply (21) with $\theta = t\log(n)$, and assume $a_n \geq 0$ for all n. The result is that all the terms in the Dirichlet series on the right are non-negative:

$$\begin{aligned} &\mathrm{Re}\left(3f(\sigma) + 4f(\sigma + it) + f(\sigma + 2it)\right) \\ &\qquad = \sum_1^\infty a_n n^{-\sigma}\left(3 + 4\cos(t\log(n)) + \cos(2t\log(n))\right) \\ &\qquad \geq 0 \; . \end{aligned}$$

This will imply that if $t \neq 0$, then

$$\lim_{\sigma \downarrow 1} \zeta(\sigma + it) \neq 0 \; . \tag{22}$$

Since $\zeta(s)$ is an analytic function (though not defined by a convergent Dirichlet series) in a neighborhood of $1+it$ for $t \neq 0$, this is the same as saying $\zeta(1+it) \neq 0$ if $t \neq 0$.

Here is one version of the argument, which is in almost every reference. It starts from the observation that $f(s) = \log(\zeta(s))$ is defined by a Dirichlet series with non-negative coefficients. The series converges for $\sigma > 1$. It comes from the Euler product and Exercise 6:

$$\zeta(s) = \prod_p \left(1 - p^{-s}\right)^{-1}$$

so

$$\begin{aligned}\log(\zeta(s)) &= -\sum_p \log(1 - p^{-s}) \\ &= \sum_p \sum_k \frac{1}{k} p^{-ks} \\ &= \sum_1^{\infty} M(n) n^{-s} \ .\end{aligned}$$

Here, $M(n)$ (for von Mangoldt) is similar to $\Lambda(n)$:

$$M(n) = \begin{cases} \frac{1}{k} & \text{if } n = p^k \text{ for some } p \\ 0 & \text{if } n \text{ has more than one prime.} \end{cases}$$

The details aren't important here, only the fact that $M(n) \geq 0$ for all n. Therefore, if $\sigma > 1$,

$$\mathrm{Re}[3\log(\zeta(\sigma) + 4\log(\zeta(\sigma) + it) + \log(\zeta(\sigma) + 2it)] \geq 0 \ .$$

We now use the fact that $|e^z| = e^{\mathrm{Re}(z)}$ and that $\zeta(\sigma)$ is real and positive (for $\sigma > 1$). Take the exponential of the log inequality and you get

$$\zeta(\sigma)^3 \left|\zeta(\sigma + it)\right|^4 \left|\zeta(\sigma + 2it)\right| \geq 1 \ . \tag{23}$$

The argument from here to the non-vanishing of $\zeta(1+it)$ uses some complex analysis. We will take the limit $\sigma \downarrow 1$ and get a contradiction if $\zeta(1 + it) = 0$. First (this isn't complex analysis) we have the bound

$$\zeta(\sigma) \leq (\sigma - 1)^{-1} + C \ .$$

If $\zeta(1+it) = 0$, then $|\zeta(\sigma + it)| \leq C\,(\sigma - 1)$. This is because $\zeta(s)$ is an analytic function of s near $s = 1 + it$. If $\zeta(1 + it) = 0$, then at least one term in the Taylor series about $1 + it$ vanishes, so $\zeta(s - (1 + it)) = O(|s - (1 + it)|^r$, where r is the order of the zero. Finally, $|\zeta(\sigma + 2it)| \leq C$, because ζ is analytic at $1 + 2it$. Altogether, we have (because $4 > 3$)

$$\zeta(\sigma)^3 \left|\zeta(\sigma + it)\right|^4 \left|\zeta(\sigma + 2it)\right| \leq C\,(\sigma - 1) \ .$$

This contradicts the inequality (23) and proves that $\zeta(1 + it) \neq 0$.

Here is another version of this argument (found in the lecture notes of Elkes) that seems to show off complex analysis in a deeper way. It starts with the non-negative Dirichlet series (15) (the minus sign in (15) gives "$\leq$" here). Therefore

$$3\frac{\zeta'(\sigma)}{\zeta(\sigma)} + 4\,\mathrm{Re}\left(\frac{\zeta'(\sigma+it)}{\zeta(\sigma+it)}\right) + \mathrm{Re}\left(\frac{\zeta'(\sigma+2it)}{\zeta(\sigma+2it)}\right) \leq 0 \; .$$

Now do Exercise 7. If $\zeta(1+it) = 0$, and it's a zero of order r, then this becomes

$$\frac{-3}{\sigma-1} + \frac{4r}{\sigma-1} + \frac{s}{\sigma-1} + O(1) \leq 0 \; ,$$

where s is the order of the possible zero of $\zeta(1+2it)$. This is not possible as $\sigma \downarrow 1$ if $r > 0$. We again used the fact that $\zeta(\sigma)$ has a simple pole as $\sigma \downarrow 1$.

5 Functional equation for ζ

The *functional equation* for $\zeta(s)$ is a relationship between $\zeta(s)$ and $\zeta(1-s)$. It is not strictly necessary to prove the prime number theorem, the books by Jameson and Apostol don't have it. But it is the basis for much of our understanding of the Riemann zeta function, which is possibly more interesting than the prime number theorem itself.

The *gamma function* is an ingredient in the functional equation for ζ. It may be defined by the integral

$$\Gamma(s) = \int_0^\infty e^{-x} x^s \frac{dx}{x} \; . \tag{24}$$

The integral converges absolutely for $s = \sigma + it$ with $\sigma > 0$. The gamma function is a generalization of the factorial function in the sense that

$$\Gamma(n) = (n-1)! \; ,$$

as you can prove by induction on n starting with $\Gamma(2) = \Gamma(1) = 1$ and

$$\Gamma(s+1) = s\Gamma(s) \; .$$

This formula is proven using integration by parts. It works for $s = \sigma + it$, as you should check. It may be written as a formula for $\Gamma(s)$ in terms of $\Gamma(s+1)$

$$\Gamma(s) = \frac{1}{s}\,\Gamma(s+1) \; . \tag{25}$$

This provides an analytic continuation of Γ first to $\sigma + it$ for $\sigma > -1$. Apply it again and you get Γ for $\sigma > -2$, and so on. The analytic continuation has a simple pole at $s = 0$ with residue 1. We can iterate to get

$$\Gamma(s) = \frac{1}{s}\frac{1}{s+1}\Gamma(s+2) \; .$$

If you take s near -1, then $s+1$ is near 0. This shows that $\Gamma(s)$ has a simple pole at $s=-1$ with residue -1.

The functional equation involves

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

The functional equation is simply

$$\xi(s) = \xi(1-s) \ . \tag{26}$$

The other special function involved in the functional equation, although it does not appear in the functional equation itself, is a *Jacobi theta function* (Jacobi defined several types of theta functions. This is just one.)

$$\theta(\tau) = \sum_{-\infty}^{\infty} e^{-\pi\tau n^2} \ . \tag{27}$$

The sum converges absolutely if $x > 0$. Later in the class we will prove the Jacobi theta function identity

$$\theta(\tau^{-1}) = \tau^{\frac{1}{2}}\theta(\tau) \ . \tag{28}$$

The theta function is related to the gamma and zeta functions through the following calculation. You do a change of variables $u = a\tau$, which is $\tau = a^{-1}u$ and $\tau^s = a^{-s}u^s$. The form $d\tau/\tau$ is convenient because $d\tau/\tau = du/u$.

$$\int_0^\infty e^{-a\tau}\tau^s \frac{d\tau}{\tau} = a^{-s}\int_0^\infty e^{-u}u^s \frac{du}{u} = a^{-s}\Gamma(s) \ .$$

We apply this to a typical term in theta function series (27). We use $\tau^{s/2}$ in order to get n^{-s} in the end:

$$\int_0^\infty e^{-\pi n^2\tau}\tau^{s/2}\frac{d\tau}{\tau} = \pi^{-\frac{s}{2}}\Gamma(\tfrac{s}{2})n^{-s} \ .$$

The theta function series may be written

$$\sum_1^\infty e^{-\pi n^2\tau} = \frac{1}{2}\left(\theta(\tau)-1\right) \ .$$

If we combine these two formulas, the result is a remarkable formula of Riemann:

$$\pi^{-\frac{s}{2}}\Gamma(\tfrac{s}{2})\zeta(s) = \frac{1}{2}\int_0^\infty \left(\theta(\tau)-1\right)\tau^{s/2}\frac{d\tau}{\tau} \ . \tag{29}$$

This formula makes sense, with all sums and integrals absolutely convergent, if $s = \sigma + it$ with $\sigma > 1$. On the left, $\pi^{-\frac{s}{2}}$ is defined for any s, the Γ integral converges absolutely if $\sigma > 0$, and the Dirichlet sum for $\zeta(s)$ converges absolutely if $\sigma > 1$. On the right, $\theta(\tau) \sim \tau^{-\frac{1}{2}}$ as $\tau \to 0$ (exercise or the Jacobi formula

(28)), so the part of the integral near $\tau = 0$ converges absolutely for $\sigma > 1$. The part of the integral as $\tau \to \infty$ converges absolutely for any s since $\theta(\tau) - 1$ goes to zero exponentially. To summarize: we have a remarkable formula, but so far it applies only where $\zeta(s)$ was defined already.

The path to the functional equation starts with some manipulations designed to broaden the range of s values where the θ integral on the right converges. The bad part is small τ, so we work on the part for $\tau \in [0, 1]$. At a crucial point, we use the Jacobi θ function identity (28).

$$\begin{aligned}
\frac{1}{2}\int_0^1 (\theta(\tau) - 1)\,\tau^{\frac{s}{2}}\,\frac{d\tau}{\tau} &= \frac{1}{2}\int_0^1 \theta(\tau)\tau^{\frac{s}{2}}\,\frac{d\tau}{\tau} + \frac{1}{2}\int_0^1 \tau^{\frac{s}{2}}\,\frac{d\tau}{\tau} \\
&= \frac{1}{2}\int_0^1 \tau^{-\frac{1}{2}}\theta(\tau^{-1})\tau^{\frac{s}{2}}\,\frac{d\tau}{\tau} + \frac{1}{2}\int_0^1 \tau^{\frac{s}{2}-1}\,d\tau \\
&= \frac{1}{2}\int_0^1 \tau^{-\frac{1}{2}}\theta(\tau^{-1})\tau^{\frac{s}{2}}\,\frac{d\tau}{\tau} + \frac{1}{s}\ .
\end{aligned}$$

You might ask why we didn't combine exponents in the first integral on the right to get $\tau^{\frac{s-3}{2}}$. That would only have made the following algebra more complicated. We use the substitution $u = \tau^{-1}$, $du = -\tau^{-2}d\tau$, $du/u = -d\tau/\tau$. Also, $\tau = u^{-1}$, so

$$\tau^{-\frac{1}{2}}\tau^{\frac{s}{2}} = u^{\frac{1}{2}}u^{-\frac{s}{2}} = u^{\frac{1-s}{2}}\ .$$

This calculation, $\tau^{\frac{s}{2}} \to u^{\frac{1-s}{2}}$, is the essence of the functional equation (26). The range of u is $1 \leq u < \infty$. We lose the minus sigh in $du/u = -d\tau/\tau$ because the direction of integration is reversed:

$$\frac{1}{2}\int_0^1 \tau^{-\frac{1}{2}}\theta(\tau^{-1})\tau^{\frac{s}{2}}\,\frac{d\tau}{\tau} = \frac{1}{2}\int_1^\infty \theta(u)u^{\frac{1-s}{2}}\,\frac{du}{u}\ .$$

This still converges only for $\sigma > 1$. The range of convergence is extended by adding and subtracting 1 from the integrand. This helps because $\theta(u) - 1$ goes to zero exponentially as $u \to \infty$ and because the pure u integral may be done analytically.

$$\frac{1}{2}\int_1^\infty \theta(u)u^{\frac{1-s}{2}}\,\frac{du}{u} = \frac{1}{2}\int_1^\infty (\theta(u) - 1)\,u^{\frac{1-s}{2}}\,\frac{du}{u} + \frac{1}{2}\int_1^\infty u^{\frac{1-s}{2}}\,\frac{du}{u}\ .$$

The second integral on the right may be done analytically:

$$\begin{aligned}
\frac{1}{2}\int_1^\infty u^{\frac{1-s}{2}}\,\frac{du}{u} &= \frac{1}{2}\int_1^\infty u^{\frac{1-s}{2}-1}\,du \\
&= \frac{1}{2}\frac{2}{1-s} \\
&= \frac{1}{1-s}\ .
\end{aligned}$$

We combine these computations and use τ for u (We'll see why right away):

$$\frac{1}{2}\int_0^1 (\theta(\tau)-1)\,\tau^{\frac{s}{2}}\,\frac{d\tau}{\tau} = \frac{1}{s} + \frac{1}{1-s} + \frac{1}{2}\int_1^\infty (\theta(\tau)-1)\,\tau^{\frac{1-s}{2}}\,\frac{d\tau}{\tau}\ .$$

The integral on the right converges absolutely for any s.

We get the functional equation using this and (29):

$$\begin{aligned}
\pi^{-\frac{s}{2}}\Gamma(\tfrac{s}{2})\zeta(s) &= \frac{1}{2}\int_0^\infty (\theta(\tau)-1)\,\tau^{s/2}\,\frac{d\tau}{\tau} \\
&= \frac{1}{2}\int_0^1 (\theta(\tau)-1)\,\tau^{s/2}\,\frac{d\tau}{\tau} + \frac{1}{2}\int_1^\infty (\theta(\tau)-1)\,\tau^{s/2}\,\frac{d\tau}{\tau} \\
&= \frac{1}{s} + \frac{1}{1-s} \\
&\quad + \frac{1}{2}\int_1^\infty (\theta(\tau)-1)\,\tau^{\frac{1-s}{2}}\,\frac{d\tau}{\tau} + \frac{1}{2}\int_1^\infty (\theta(\tau)-1)\,\tau^{s/2}\,\frac{d\tau}{\tau}\ .
\end{aligned}$$

Now we're there. The integrals on the right make sense for any s (except possibly the poles $s=0$ and $s=1$). The right side is clearly symmetric: if you replace s by $1-s$, the formula is the same. Riemann was looking for a way to get around the divergence of the Dirichlet series near $s=1$ and found not only an analytic continuation of $\zeta(s)$, but a remarkable symmetry.

5.1 Theta functions and the heat equation

The theta function identity (28) looks surprising and strange. You should wonder how anyone could discover such a formula, let alone prove it. I don't know how it was discovered. But I know a way it could have been discovered in around 1820 (about the time it was discovered). It arises naturally from two ways to solve the heat equation, both of which were developed by Fourier and others around this time. Pure mathematicians often brag about all the things they discovered while pursuing pure thought questions with no obvious applications. They have a point. But they should acknowledge that many of the facts they work with were discovered by applied mathematicians and scientists with specific applications in mind.

The *heat equation* is a partial differential equation for a function $u(x,t)$ defined for $t \geq 0$. The function u represents the temperature at a point x at time t. At the "initial time", $t=0$ we have an "initial condition", which is the temperature profile $u(x,0)$. The temperature profile at later times, $t>0$ is determined by the initial condition and "heat flow". The physical hypothesis is that heat flows from high temperature to low temperature. There is a *heat flux*, F, which is proportional to the temperature gradient

$$F(x,t) = -D\frac{\partial u(x,t)}{\partial x}$$

This formula is *Fick's law* and D is the *diffusion coefficient* (diffusion being another way of thinking about heat flow). The amount of heat in the interval

$[a,b]$ at time t is

$$\int_a^b u(x,t)\,dx\ .$$

The rate of change of this amount is given by the heat flux at the ends:

$$\frac{d}{dt}\int_a^b u(x,t)\,dx = -F(b,t) + F(a,t)\ .$$

If u is decreasing as a function of x at b and t, then the heat is flowing from the warmer part ($x < b$) to the colder part ($x > b$). The flux formula (Fick's law) makes $F(b,t) > 0$ there. This makes the heat in $[a,b]$ decrease (check the three minus signs resulting in an overall negative – $\partial u/\partial x < 0$ implies $F > 0$, which implies that $-F < 0$. Similar reasoning applies at $x = a$, but here $F > 0$ is heat flowing into $[a,b]$.

We derive a partial differential equation for u from these formulas. First,

$$\begin{aligned}-F(b,t) + F(a,t) &= D\left(\frac{\partial u(b,t)}{\partial x} - \frac{\partial u(a,t)}{\partial x}\right)\\ &= D\int_a^b \frac{\partial u^2}{\partial^2 x}\ .\end{aligned}$$

Next,

$$\frac{d}{dt}\int_a^b u(x,t)\,dx = \int_a^b \frac{\partial u(x,t)}{\partial t}\,dt\ .$$

If these formulas hold for every $a < b$ and every $t > 0$, and if the partial derivatives in the formulas are continuous functions of x and t, then the equality must apply "pointwise" for every x and $t > 0$:

$$\frac{\partial u}{\partial t} = D\frac{\partial u^2}{\partial^2 x}\ . \tag{30}$$

You can get some intuition for the heat equation by asking what happens at a local maximum or minimum of u as a function of x. At a local maximum (as a function of x), the right side of (30) is negative, so u is decreasing (as a function of t) – heat flows away from a hot-spot, so the temperature there goes down. Similarly, the temperature increases at a local minimum.

The *fundamental solution* to the heat equation is the function

$$u(x,t) = \frac{1}{\sqrt{4\pi Dt}}e^{-\frac{x^2}{4Dt}}\ . \tag{31}$$

You can check directly that this satisfies the heat equation. We may leave out the constant $(4\pi D)^{-1/2}$.

$$t^{-\frac{1}{2}}e^{-\frac{x^2}{4Dt}} \xrightarrow{\frac{\partial}{\partial t}} -\frac{1}{2}t^{-\frac{3}{2}}e^{-\frac{x^2}{4Dt}} + t^{-\frac{1}{2}}\frac{x^2}{4Dt^2}e^{-\frac{x^2}{4Dt}}\ .$$

Also

$$t^{-\frac{1}{2}}e^{-\frac{x^2}{4Dt}} \xrightarrow{\frac{\partial}{\partial x}} -t^{-\frac{1}{2}}\frac{x}{2Dt}e^{-\frac{x^2}{4Dt}} \xrightarrow{\frac{\partial}{\partial x}} -t^{-\frac{1}{2}}\frac{1}{2Dt}e^{-\frac{x^2}{4Dt}} + t^{-\frac{1}{2}}\frac{x^2}{4D^2t^2}e^{-\frac{x^2}{4Dt}} \ .$$

You can see from these calculations that $\partial u/\partial t$ is indeed equal to $D\partial^2 u/\partial x^2$. It is possible to derive this formula without any great brilliance or guesswork using the Fourier transform. In fact, Fourier seems to have invented the Fourier transform for this purpose. In French speaking countries, what was called Fick's law is often called the *Fourier law*. Fourier was interested in heat flow.

The solution (31) is called "fundamental" because it is the solution that results from the initial condition of a unit amount of heat concentrated at $x = 0$. We write $u(x, 0) = \delta(x)$. This is informal, because $t = 0$ in (31) makes no literal sense. The total amount of heat is

$$\int_{-\infty}^{\infty} u(x,t)\,dx \ .$$

You can show this is constant by differentiating with respect to t and using the heat equation to turn that to an x derivative (and $u \to 0$ strongly as $x \to \pm\infty$). Therefore, you can check the integral by choosing any t value you like, such as the t value that makes $4Dt = 1$. Then

$$\int_{-\infty}^{\infty} u(x,t)\,dx = \frac{1}{\sqrt{\pi}}\int_{-\infty}^{\infty} e^{-x^2}\,dx = \frac{1}{\sqrt{\pi}}\sqrt{\pi} = 1 \ .$$

As $t \downarrow 0$, all this mass accumulates at the point $x = 0$. For example, for any $\epsilon > 0$,

$$\int_{|x|>\epsilon} u(x,t)\,dx \to 0 \ , \quad \text{as } t \downarrow 0$$
$$\int_{|x|\le\epsilon} u(x,t)\,dx \to 1 \ , \quad \text{as } t \downarrow 0 \ .$$

Physicists picture the δ function the limit of this process − all it's mass at $x = 0$. This solution is "fundamental" because you can make any other solution in terms of this one. See any good book on partial differential equations or heat flow for an explanation.

Fourier also was interested in periodic heat distributions. These satisfy $u(x + 1, t) = u(x, t)$ for all x and all $t > 0$. You could consider (but we don't here) periodic solutions that satisfy $u(x_L, t) = u(x, t)$. These repeat themselves every L units of x rather than every one unit of x. The periodic function that plays the role of fundamental solution is

$$u(x,t) = \sum_{-\infty}^{\infty} u_f(x-n,t) = \frac{1}{\sqrt{4\pi Dt}}\sum_{-\infty}^{\infty} e^{-\frac{(x-n)^2}{4Dt}} \ .$$

If you take $x = 0$ and t so that

$$4\pi Dt = \tau \ , \tag{32}$$

this sum is

$$\tau^{-\frac{1}{2}} \sum_{-\infty}^{\infty} e^{\frac{-\pi n^2}{\tau}} \ .$$

This looks encouraging for (28).

Fourier invented or knew another way to express the solution of the heat equation for periodic functions – Fourier series. The solution may be written in the form

$$u(x,t) = \sum_{-\infty}^{\infty} \widehat{u}_n(t) e^{2\pi i n x} \ . \tag{33}$$

The functions $e^{2\pi i n x}$ are periodic with period 1. As we saw in the discrete Fourier transform, any periodic function may be written as a sum of these periodic functions – they form a basis of the space of periodic functions. The initial condition

$$u(x,0) = \sum_n \delta(x-n)$$

gives an initial condition on the Fourier coefficients (we will see)

$$\widehat{u}_n(0) = 1 \ .$$

The heat equation gives

$$\sum_{-\infty}^{\infty} \left(\frac{d}{dt} \widehat{u}_n(t) \right) e^{2\pi i n x} = D \sum_{-\infty}^{\infty} \widehat{u}_n(t) \left(-4\pi^2 n^2 \right) e^{2\pi i n x} \ .$$

We equate the coefficients of $e^{2\pi i n x}$ and get

$$\frac{d}{dt} \widehat{u}_n(t) = -4D\pi^2 n^2 \widehat{u}_n(t) \ .$$

The solution of this differential equation, with the initial condition above, is

$$\widehat{u}_n(t) = e^{-4Dn^2\pi^2 t} \ .$$

Therefore,

$$u(x,t) = \sum_{-\infty}^{\infty} e^{-4Dn^2\pi^2 t} e^{2\pi i n x} \ .$$

Finally, we set $x = 0$ and choose t as before (32). The result is

$$u(0,t) = \sum_{-\infty}^{\infty} e^{-n^2 \pi \tau} \ .$$

The two formulas for $u(0,t)$ lead to

$$\sum_{-\infty}^{\infty} e^{-n^2\pi\tau} = \tau^{-\frac{1}{2}} \sum_{-\infty}^{\infty} e^{\frac{-\pi n^2}{\tau}} \ . \tag{34}$$

This is the Jacobi theta function identity (28).

The two sides of (34) are useful for different ranges of τ. For large τ, the left side converges quickly and the right side converges slowly. For small τ, it goes the other way. There is more about theta functions in the exercises.

6 Exercises

1. Consider the Dirichlet series

$$f(s) = \sum_1^\infty a_n n^{-s} .$$

The partial sums of the coefficients are

$$A_n = \sum_1^n a_k .$$

(a) Show that if the partial sums are bounded (there is a C with $A_n \leq C$ for all n), then the Dirichlet series converges for $s = \sigma + it$ and $\sigma > 0$. *Hint*: use Abel summation.

(b) Use part (a) to show that the non-principal L functions are analytic (with no pole at $s = 1$).

(c) Suppose $a_n = \pm 1$ with the sign chosen independently, at random, with $\Pr(a_n = 1) = \Pr(a_n = -1) = \frac{1}{2}$. It is known that for any $\epsilon > 0$, then *almost surely* (with probability 1)

$$\max_n \frac{|A_n|}{n^{\frac{1}{2}+\epsilon}} < \infty .$$

Use this to show that $f(s)$ is analytic for $\sigma > \frac{1}{2}$, again with no pole at $s = 1$.

2. (*Stirling's approximation*) We want to approximate

$$\sum_{k=2}^n \log(k)$$

by an integral like

$$\int_2^n \log(y)\, dy = n \log(n) - n + O(??) .$$

The key step is a bound on the error over one "panel":

$$\left| \log(k) - \int_k^{k+1} \log(y)\, dy \right| \leq ?? .$$

(a) Show that if $k \le y \le k+1$, then

$$|\log(y) - \log(k)| \le \frac{1}{k} \ .$$

You can do this using just calculus (the intermediate value theorem) or slopes and geometry.

(b) Show that

$$\sum_1^n \frac{1}{k} = O(\log(n)) \ .$$

(c) Use this to verify the Stirling approximation (10) for integer x.

(d) Verify the full approximation (10) for non-integer x. You can do this by asking how $x\log(x)-x$ varies in the interval $[n, n+1]$, or by asking how large the fractional contribution $\int_n^{x-n} \log(y)\,dy$ can be.

3. Here is another way to get information about prime numbers from $n!$. For this, we write $[x]$ for the *integer part* of x, which is the largest integer $\le x$. For example $[\pi] = 3$, and $[\frac{n}{2}] = n/2$ if and only if n is even (n being a positive integer).

(a) Show that

$$\log(n!) = \sum_{p \le n} \left[\frac{n}{p}\right] \log(p) \ .$$

(b) Show that

$$\left| \sum_{p \le n} \left(\frac{n}{p} - \left[\frac{n}{p}\right] \right) \log(p) \right| = O(n) \ .$$

Hint: Use one of the Chebychev bounds.

(c) Show that

$$\sum_{p \le n} \frac{\log(p)}{p} = \log(n) + O(1) \ . \tag{35}$$

This is called *Mertens' theorem*. *Hint*: Combine parts (a) and (b) with Stirling's approximation.

(d) Use Abel summation to show that Mertens' theorem (35), but with $o(\log(n))$ instead of $O(1)$ as the error bound, is a consequence of the prime number theorem in the form $\pi(n) = n/\log(n) + o(n/\log(n))$.

(e) (Harder, do as time permits.) Show that the converse is not true. Show that there is a set of positive integers Q so that

$$\lambda(n) = \sum_{q \le n, q \in Q} \frac{\log(q)}{q} = \log(n) + O(1) \ ,$$

But the "prime number theorem" for Q is false, which would be

$$\sum_{q \le n, q \in Q} 1 = \frac{n}{\log(n)} + o\left(\frac{n}{\log(n)}\right) .$$

That is, if

$$\rho(x) = \sum_{q \le n, q \in Q} 1 ,$$

then

$$\lim_{x \to \infty} \frac{\log(x)}{x} \rho(x)$$

does not exist.

4. Use the arguments leading to (20) to find a bound of the form

$$|\zeta'(1 + it)| = O(\log^p(|t|)) \ , \quad \text{as} \ \ |t| \to \infty \ .$$

5. Use the arguments leading to (20) to find a bound of the form

$$\left|\zeta(\frac{1}{2} + it)\right| = O(|t|^p) \ , \quad \text{as} \ \ |t| \to \infty \ .$$

   Your best bound may be of the form: "any $p > p_0$", though you can't do it for p_0. The conjecture that any $p > 0$ works is the *Lindelöf* conjecture. Don't expect to prove it.

6. Show that if $|x| < 1$ then

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

   This is a calculus exercise in Taylor series. Make a simple argument that the signs are right (minus on the left, all positive on the right).

7. Suppose $f(z)$ in analytic in a neighborhood of z_0 and f has a zero of order r at z_0. Show that

$$\frac{f'(z)}{f(z)} = \frac{r}{z - z_0} + O(1) \ , \quad \text{as} \ z \to z_0 \ .$$

8. Show that $\Gamma(\sigma + it) \to 0$ as $t \to \infty$ if $\sigma > 0$. *Hint*: use the recurrence relation (25) and the integral representation (24).

9. Show that the recurrence relation (25) defines a function $\Gamma(s)$ in the whole complex plane, except for isolated poles. A function like this is called *meromorphic*. Show that the only poles of $\Gamma(s)$ are simple poles at $s = -n$ for $n \ge 0$. Find the residue at $s = -n$.

10. Show that $\theta(\tau) - 1 = O(e^{-\pi\tau})$ as $\tau \to \infty$.

11. Consider the fake theta function sum

$$\sigma(\tau) = \sum_{n=-\infty}^{\infty} e^{-\tau n^4} \ .$$

Show that $\sigma(\tau) = A\tau^{-\frac{1}{4}} + O(1)$ as $\tau \to 0$. Write an integral formula for A. *Hint:* For small τ, either (n not too large, depending on τ)

$$e^{-\tau n^4} = \int_n^{n+1} e^{-\tau x^4}\, dx + (\text{smaller}) \ ,$$

or $e^{-\tau n^4}$ is very small and rapidly decreasing (n large, depending on τ).

12. Show that $\theta(\tau) = \tau^{-\frac{1}{2}} + O(1)$ as $\tau \to 0$.

    (a) Do this using the method of exercise 11.

    (b) Do this using the Jacobi theta function identity.

13. The Euler/Riemann version of the Γ function is

$$\Pi(s) = \int_0^\infty x^{-s} e^{-s}\, dx = \int_0^\infty e^{\phi(x,s)}\, dx \ , \quad \phi(x,s) = s\log(x) - x \ . \qquad (36)$$

Clearly $\Pi(s-1) = \Gamma(s)$, so you use one or the other for convenience. This exercise studies the behavior of $\Pi(s)$ for large real s, which we emphasize by writing σ for s. The *Laplace method* is a way to find Stirling's approximation to $\Pi(\sigma)$ as the real variable σ goes to infinity. It is based on two observations: (1) "most" of the integral (36) comes from a small neighborhood of x_*, which is where ϕ is maximized, and (2) the Taylor series $\phi(x,\sigma) \approx \phi(x_*,\sigma) - \frac{H}{2}(x-x_*)^2$ is accurate in such a small neighborhood. The approximation is

$$\Pi(\sigma) = A(\sigma)\sigma^\sigma e^{-\sigma} \ , \qquad (37)$$

where the amplitude (hence "A") *prefactor* is

$$A(\sigma) = \sqrt{2\pi\sigma} + O(\sigma^{-\frac{1}{2}}) \ .$$

(We've had all this before, except that it was only for integers $\sigma = n$ and we didn't know the constant $\sqrt{2\pi}$.)

   (a) Identify x_* as a function of σ. Calculate H as a function of σ. Define $\psi = \phi(x_*,\sigma) - \frac{H}{2}(x-x_*)^2$ and write an error bound (inequality showing $\phi \approx \psi$) involving a power of σ and $\left|x - x_*\right|^3$ that should hold near x_*.

   (b) Find a number $r(\sigma)$ so that

(1)	$\int_0^r e^{\phi(x,\sigma)}\, dx = o(\Pi(\sigma))$
(2)	$\left\lvert e^{\phi(r,\sigma)} - e^{\psi(r,\sigma)} \right\rvert = o(e^{\phi(r,\sigma)})$

(c) Find a number $R(s)$ so that

$$
\begin{array}{ll}
(1) & \int_R^\infty e^{\phi(x,\sigma)}\,dx = o(\Pi(\sigma)) \\
(2) & \left|e^{\phi(R,\sigma)} - e^{\psi(R,\sigma)}\right| = o(e^{\phi(R,\sigma)})
\end{array}
$$

Hint: The simplest thing is $r = x_* - s^{-\alpha}$ and $R = x_* + s^{-\alpha}$, with α an appropriately chosen fraction.

(d) Show that

$$\left|e^{\phi(x,\sigma)} - e^{\psi(x,\sigma)}\right| = o(e^{\phi(x,\sigma)}) ,$$

for $r \leq s \leq R$.

(e) Finish the proof of (37).

14. Derive the infinite product representation

$$\Gamma(s) = \frac{1}{s}\prod_1^\infty \left[\left(1+\frac{s}{n}\right)^{-1} e^{\frac{s}{n}}\right]$$

(a) Show that as long as $s \notin \{0, -1, -2, \ldots\}$ then the infinite product converges absolutely.

(b) Assuming that the formula is true, use it to show that $\Gamma(s) \neq 0$ for all s.

(c) Derive the formula

$$\Gamma(s) = \left[\prod_0^n (s+k)^{-1}\right]\Gamma(s+n+1) .$$

(d) Assume Stirling's approximation in the form

$$\Gamma(s) = A(s)s^s e^{-s} \quad , \quad \text{where } \lim_{n\to\infty}\frac{A(s+n)}{A(n)} = 1 \text{ for any } s.$$

Use this to derive the infinite product representation. This is most of the work and takes a lot of careful algebra and analytic reasoning. Please do it carefully and write it up in a way that makes the steps clear and easy to read. This problem will be graded for clarity as well as correctness.