On a numerical upper bound for the extended Goldbach conjecture

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Declaration

The work in this thesis is my own except where otherwise stated.

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I wish to thank my supervisor Tim Trudgian. His advice and weekly meetings provided much needed support whenever I'd get stuck on a problem or become disheartened. I find myself in the most fortunate position of finishing honours in mathematics with the same person as when I started it, way back in 2013 when I took MATH1115.[1]

Having the most engaging lecturer during my first year of undergraduate helped to foster my interest in mathematics, and I've yet to see any other lecturer at this university take the time to write letters of congratulations to those that did well in their course.

[1] I still remember the hilarious anecdote in class about cutting a cake "coaxially".

Abstract

The Goldbach conjecture states that every even number can be decomposed as the sum of two primes. Let $D(N)$ denote the number of such prime decompositions for an even N. It is known that $D(N)$ can be bounded above by

$$D(N) \leq C^* \frac{N}{\log^2 N} \prod_{\substack{p \mid N \\ p>2}} \left(1 + \frac{1}{p-2}\right) \prod_{p>2} \left(1 - \frac{1}{(p-1)^2}\right) = C^* \Theta(N)$$

where C^* denotes Chen's constant. It is conjectured [20] that $C^* = 2$. In 2004, Wu [54] showed that $C^* \leq 7.8209$. We attempted to replicate his work in computing Chen's constant, and in doing so we provide an improved approximation of the Buchstab function $\omega(u)$,

$$\begin{aligned} \omega(u) &= 1/u, \quad (1 \leq u \leq 2), \\ (u\omega(u))' &= \omega(u-1), \quad (u \geq 2). \end{aligned}$$

based on work done by Cheer and Goldston [6]. For each interval $[j, j+1]$, they expressed $\omega(u)$ as a Taylor expansion about $u = j+1$. We expanded about the point $u = j + 0.5$, so $\omega(u)$ was never evaluated more than 0.5 away from the center of the Taylor expansion. which gave much stronger error bounds.

Issues arose while using this Taylor expansion to compute the required integrals for Chen's constant, so we proceeded with solving the above differential equation to obtain $\omega(u)$, and then integrating the result. Although the values that were obtained undershot Wu's results, we pressed on and refined Wu's work by discretising his integrals with finer granularity. The improvements to Chen's constant were negligible (as predicted by Wu). This provides experimental evidence, but not a proof, that were Wu's integrals computed on smaller intervals in exact form, the improvement to Chen's constant would be similarly negligible. Thus, any substantial improvement on Chen's constant likely requires a radically different method to what Wu provided.

Contents

Notation and terminology

In the following, p, q usually denote primes.

Notation

GRH	Generalised Riemann hypothesis.
TGC	Ternary Goldbach conjecture.
GC	Goldbach conjecture.
FTC	Fundamental theorem of calculus.
$f(x) \ll g(x)$	g is an asymptotic upper bound for f, that is, there exists constants M and c such that for all $x > c$, $\lvert f(x)\rvert \leq M\lvert g(x)\rvert$.
$f(x) \gg g(x)$	g is an asymptotic lower bound for f, that is, there exists constants M and c such that for all $x > c$, $\lvert f(x)\rvert \geq M\lvert g(x)\rvert$. Equivalent to $g \ll f$.
$f(x) \sim g(x)$	g is an asymptotic tight bound for f, that is, $\lim\limits_{n\to\infty} \frac{f(n)}{g(n)} = 1$. Equivalent to $f \ll g$ and $g \ll f$.
C_0	Twin primes constant, §1.10
$\pi(x)$	Number of primes p less than x.
$\mathbb{P}$	Set of all primes p.
$\mathbb{P}_{\leq n}$	Set of all numbers with at most n prime factors. Also denoted $\mathbb{P}_n$ for brevity.
$S(\mathcal{A}; \mathcal{P}, z)$	Sifting function, §2.1.
$\mathcal{A}$	Set of numbers to be sifted by a sieve $S(\mathcal{A}; \mathcal{P}, z)$.

$\mathcal{A}_{\leq x}$	$\{a : a \in \mathcal{A}, a \leq x\}$.
$\mathcal{A}_d$	$\{a : a \in \mathcal{A}_{\leq x}, a \equiv 0 \bmod d\}$ for some square-free d.
$\mathbf{1}_E(x)$	Characteristic function on a set E. Equals 1 if $x \in E$, 0 otherwise.
$\mathcal{P}$	Usually denotes a set of primes.
X	Shorthand for $X(x)$, denotes the main term in an approximation to a sieve.
R	The remainder, or error term, for an approximation to a sieve.
C^*	Chen's constant, §1.8.
$\omega(u)$	Buchstab's function, §4.1.
γ	Euler–Mascheroni constant.
$\mu(x)$	Möbius function.
$\varphi(n)$	Euler totient function.
K	Linnik–Goldbach constant, §1.9.
$\#A$	The cardinality of the set A.
(a, b)	Greatest common divisor of a and b. Sometimes denoted $\gcd(a, b)$ if (a, b) is ambiguous and could refer to an ordered pair.
$\operatorname{lcm}(a, b)$	Least common multiple of a and b.
$f * g$	Dirichlet convolution of f and g, defined as $(f * g)(x) = \sum_{d\mid n} f(d)g(n/d)$
$a \mid b$	a divides b, i.e. there exists some n such that $b = na$.
$a \nmid b$	a does not divide b
$\operatorname{Li}(x)$	Logarithmic integral, $\operatorname{Li}(x) = \int_2^x \frac{1}{\log t}\, dt$

Chapter 1

History of Goldbach problems

1.1 Origin

One of the oldest and most difficult unsolved problems in mathematics is the Goldbach conjecture (sometimes called the Strong Goldbach conjecture), which originated during correspondence between Christian Goldbach and Leonard Euler in 1742. The Goldbach conjecture states that "Every even integer $N > 2$ can be expressed as the sum of two primes" [17].
For example,

$$4 = 2 + 2 \qquad 8 = 5 + 3 \qquad 10 = 7 + 3 = 5 + 5.$$

Evidently, this decomposition need not be unique. The Goldbach Conjecture has been verified by computer search for all even $N \leq 4 \times 10^{18}$ [12], but the proof for all even integers remains open.* Some of the biggest steps towards solving the Goldbach conjecture include Chen's theorem [44] and the Ternary Goldbach conjecture [23].

1.2 Properties of $D(N)$

As the Goldbach conjecture has been unsolved for over 250 years, a lot of work has gone into solving weaker statements, usually by weakening the statement that N is the sum of two primes. Stronger statements have also been explored. We define $D(N)$ as the number of ways N can be decomposed into the sum of two primes. The Goldbach conjecture is then equivalent to $D(2N) \geq 1$ for all

*Weakening Goldbach to be true for only sufficiently large N is also an open problem.

N. As N grows larger, more primes exist beneath N (approximately $\frac{N}{\log N}$ many, from the prime number theorem) that could be used to construct a sum for N. Thus, we expect large numbers to have many prime decompositions. And indeed empirically this seems to be the case.

Below are some examples of prime decompositions of even numbers.

$$
\begin{aligned}
36 &= 31 + 5 & 66 &= 61 + 5 & 90 &= 83 + 7 & &= 61 + 29 \\
&= 29 + 7 & &= 59 + 7 & &= 79 + 11 & &= 59 + 31 \\
&= 23 + 13 & &= 53 + 13 & &= 73 + 17 & &= 53 + 37 \\
&= 19 + 17 & &= 47 + 19 & &= 71 + 13 & &= 47 + 43 \\
& & &= 43 + 23 & &= 67 + 23 & & \\
& & &= 37 + 29 & & & &
\end{aligned}
$$

Intuitively, we would expect that as N grows large, $D(N)$ should likewise grow large. The extended Goldbach conjecture [20] asks how $D(N)$ grows asymptotically. As expected, the conjectured formula for $D(N)$ grows without bound as N increases (Figure 1.1).

We can see from the plots that the points of $D(N)$ cluster into bands, and $2\Theta(N)$ also shares this property (Figure 1.2). The plot of $D(N)$ called "Goldbach's Comet" [14], which has many interesting properties. We plot $D(N)$, and colour each point either red, green or blue if ($N/2 \bmod 3$) is 0, 1 or 2 respectively (Figure 1.3). [14]. We can see the bands of colours are visibly separated. If $D(N)$ is plotted only for prime multiples of an even number [2], say

$$N = 12 \times 2, 12 \times 3, 12 \times 5, \ldots$$

the resulting plot is almost a straight line (Figure 1.4).

1.3 Ternary Goldbach conjecture

The Ternary Goldbach conjecture (TGC) states that "every odd integer greater than 5 can be expressed as the sum of three primes". This statement is directly implied by the Goldbach conjecture, as if every even $n > 2$ can be expressed as $n = p + q$, where p, q prime, we can express all odd integers n' greater than 5 as three primes

$$n' = n + 3 = p + q + 3.$$

In 1923, Hardy and Littlewood [20] showed that, under the assumption of the generalised Riemann hypothesis (GRH), the TGC is true for all sufficiently large

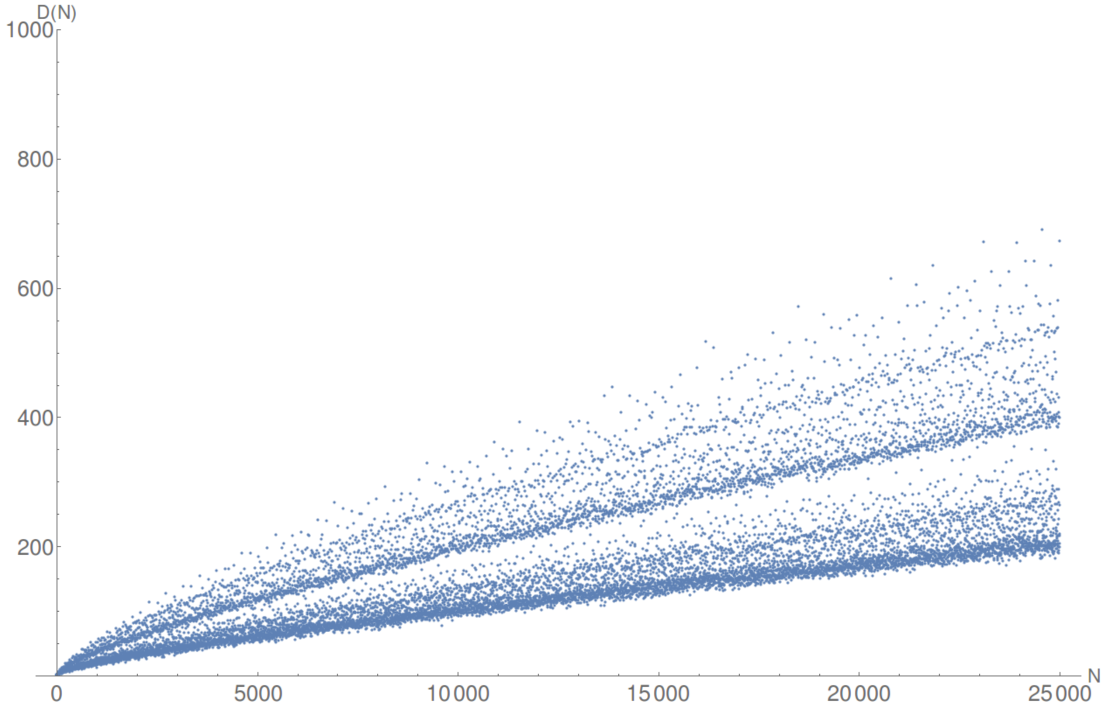


Figure 1.1: Plot of $D(N)$ for $N \leq 25000$.

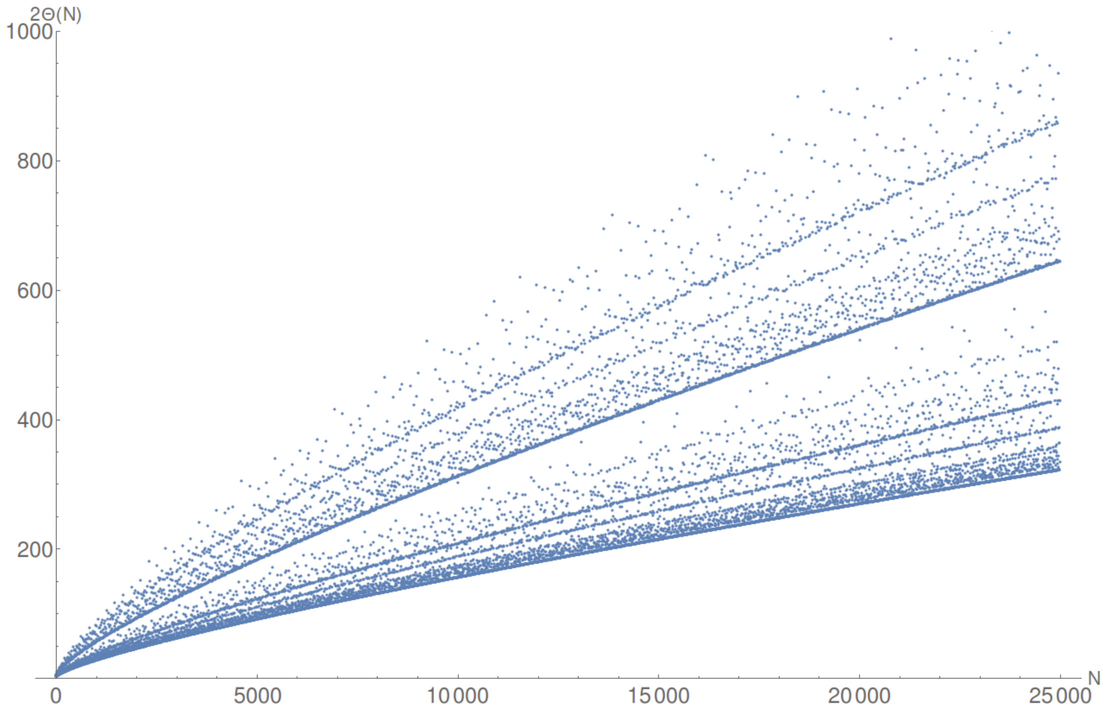


Figure 1.2: Plot of $2\Theta(N)$, the conjectured tight bound to $D(N)$, for $N \leq 25000$.

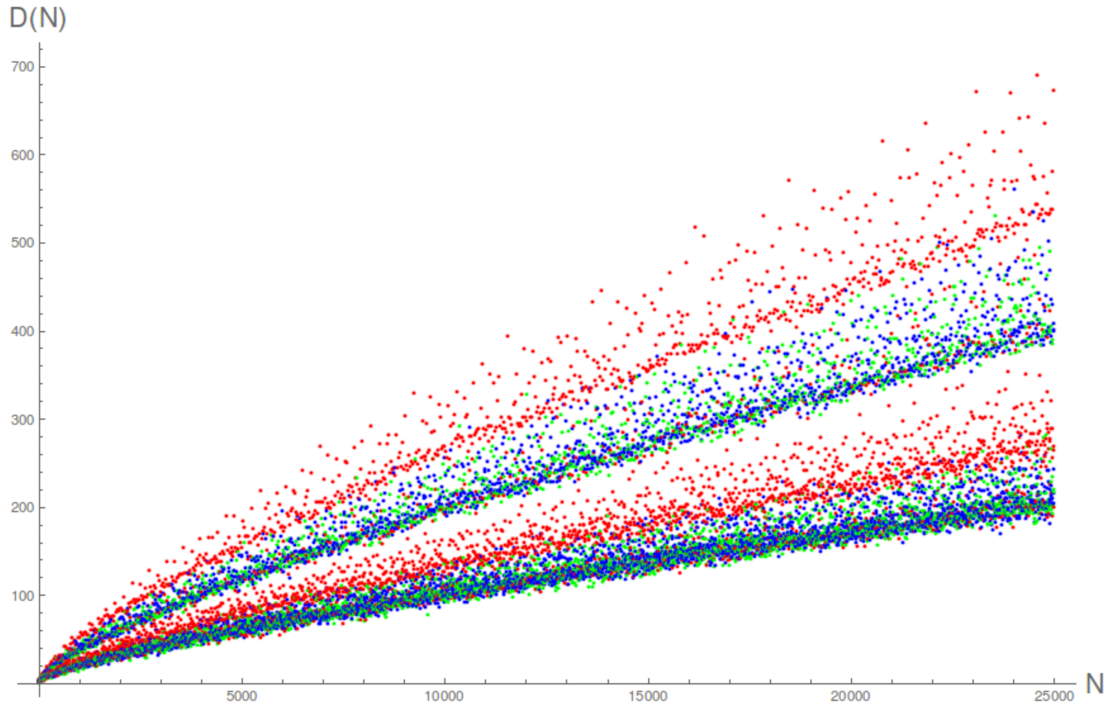


Figure 1.3: Plot of $D(N)$ for $N \leq 25000$, points coloured based on $N/2 \bmod 3$.

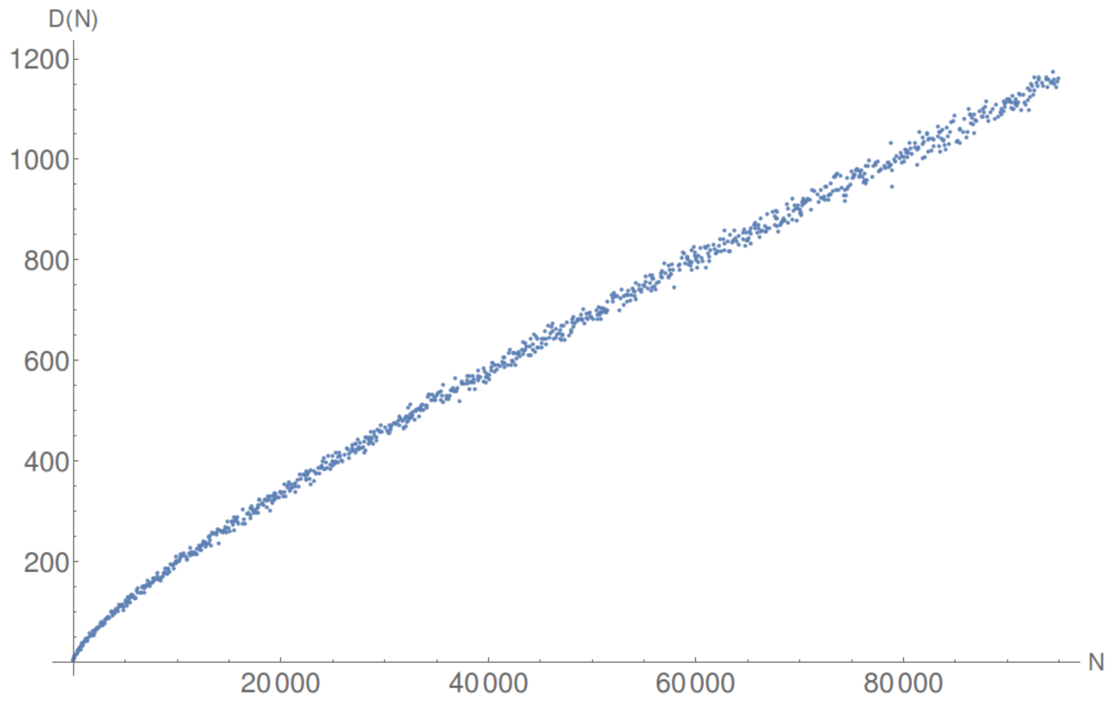


Figure 1.4: Plot of $D(N)$ restricted to $N = 12p, 12p \leq 10^5$

odd numbers. They also specified how $D_3(n)$ (the number of ways n can be decomposed as the sum of three primes) grows asymptotically

$$D_3(n) \sim C_3 \frac{n^2}{\log^3 n} \prod_{\substack{p|n \\ p \text{ prime}}} \left(1 - \frac{1}{p^2 - 3p + 3}\right), \tag{1.1}$$

where

$$C_3 = \prod_{\substack{p>2 \\ p \text{ prime}}} \left(1 + \frac{1}{(p-1)^3}\right).$$

Using the Taylor expansion of $\exp(x)$ and the fact that every term in the sum is positive, we obtain the inequality

$$1 + x \leq 1 + x + \frac{x^2}{2!} + \ldots = \sum_{n=0}^{\infty} \frac{x^n}{n!} = \exp(x).$$

Hence by induction, for all non-negative sequences $\{a_1, \ldots, a_n\}$

$$\prod_{i=1}^{n} (1 + a_i) \leq \exp\left(\sum_{i=1}^{n} a_i\right). \tag{1.2}$$

Therefore we may note that C_3 must converge, as

$$C_3 < \prod_{n \geq 2} \left(1 + \frac{1}{n^3}\right) \leq \exp\left(\sum_{n=2}^{\infty} \frac{1}{n^3}\right) < \infty.$$

We also note that the product over all primes dividing n in (1.1) grows slowly compared to the main term, as for all $n \geq 2$

$$n^2 - 3n + 3 \geq \frac{1}{2} n$$

$$1 - \frac{1}{n^2 - 3n + 3} \geq 1 - \frac{2}{n}$$

$$\prod_{\substack{p|n \\ p \text{ prime}}} \left(1 - \frac{1}{p^2 - 3p + 3}\right) \geq \prod_{\substack{p|n \\ p \text{ prime}}} \left(1 - \frac{2}{p}\right) \geq \prod_{\substack{2<p\leq n \\ p \text{ prime}}} \left(1 - \frac{2}{p}\right).$$

We have from Mertens' theorem [10] that

$$\prod_{\substack{p\leq n \\ p \text{ prime}}} \left(1 - \frac{1}{p}\right) \sim \frac{e^{-\gamma}}{\log n}. \tag{1.3}$$

Combining this with the following inequality

$$1 - \frac{2}{x} \geq \frac{1}{2}(1 - \frac{1}{x})^2 \text{ for } x \geq 3, \tag{1.4}$$

we obtain

$$\prod_{\substack{2<p\leq n\\ p\text{ prime}}}\left(1-\frac{2}{p}\right)\geq\frac{1}{2}\prod_{\substack{2<p\leq n\\ p\text{ prime}}}\left(1-\frac{1}{p}\right)^2\sim\frac{e^{-2\gamma}}{2\log^2 n},$$

which gives an asymptotic lower bound on $D_3(n)$

$$D_3(n)\gg\frac{n^2}{\log^5 n}.$$

This gives a stronger version of the TGC, as it implies that the number of different ways that an odd integer can be decomposed as the sum of three primes can be arbitrarily large. In 1937, Vinogradov improved this result by removing the dependency on GRH [50].

An explicit value for how large N needs to be before the TGC holds was found by Borozdin, who showed that $N>3^{3^{15}}$ is sufficient [16]. In 1997, the TGC was shown to be conditionally true for all odd $N>5$ by Deshouillers et al, [11] under the assumption of GRH. The unconditional TGC was further improved by Liu and Wang [34] in 2002, who showed that Borozdin's constant can be reduced to $N>e^{3100}$. Thus, in principle, all that was needed to prove the TGC was to check that it held for all $N<e^{3100}\approx 10^{7000}$. Given that the number of particles in the universe $\approx 10^{80}$, no improvements to computational power would likely help. Further mathematical work was necessary.

In 2013, Helfgott reduced the constant sufficiently as to allow computer assisted search to fill the gap, obtaining $N>10^{27}$ [23]. When combined with his work numerically verifying the TGC for all $N<8.875\times 10^{30}$, [23] Helfgott succeeded in proving the TGC.

1.4 Extended Goldbach conjecture

Hardy and Littlewood's paper [20] discuss how one can directly obtain an asymptotic formula (conditional on GRH) for the numbers of ways even N can be decomposed into the sum of four primes. Let $D_4(N)$ be the number of such ways.

$$D_4(N)\sim\frac{1}{3}C_4\frac{n^3}{\log^4 n}\prod_{\substack{p\mid n\\ p>2}}\left(1+\frac{1}{(p-2)(p^2-2p+2)}\right),\tag{1.5}$$

where

$$C_4=\prod_{p>2}\left(1-\frac{1}{(p-1)^4}\right).$$

The asymptotic formulae for $D_3(N)$ and $D_4(N)$ are very similar (checking convergence and the long term behaviour of $D_4(N)$ is the same proof as for $D_3(N)$). Hardy–Littlewood claim that one can easily generalise their work to obtain an asymptotic formula for $D_r(N)$ for $r > 2$. However, for $r = 2$, the results do not easily generalise:

> "It does not fail *in principle*, for it leads to a definite result which appears to be correct; but we cannot overcome the difficulties of the proof..."[20, p. 32]

The following asymptotic formula for $D(N)$ was thus conjectured [20]

$$D(N) \sim 2\Theta(N), \tag{1.6}$$

where

$$\Theta(N) := \frac{C_N N}{\log^2 N}, \qquad C_N := C_0 \prod_{\substack{p \mid N \\ p>2}} \left(1 + \frac{1}{p-2}\right), \quad C_0 := \prod_{p>2} \left(1 - \frac{1}{(p-1)^2}\right).$$

Now C_0 denotes the twin primes constant (see 1.10), and each term in the infinite product in C_N is greater than 1. Thus, $C_N > C_0$, which provides an asymptotic lower bound of

$$D(N) \gg \frac{N}{\log^2 N}, \tag{1.7}$$

Hence, (1.6) implies the Goldbach conjecture (for large N), which should indicate the difficulty of the problem.

There has been progress in using (1.6) as a way to construct an upper bound for $D(N)$, by seeking the smallest values of C^* (hereafter referred to as Chen's constant) such that

$$D(N) \leq C^* \Theta(N)^{\ddagger} \tag{1.8}$$

Upper bounds for C^* have been improved over the years, but recent improvements have been small[†] (see Table 1.1). Recent values have been obtained by various sieve theory methods by constructing large sets of weighted inequalities (the one in Wu's paper has 21 terms!). However, the reductions in C^* are minuscule. One would suspect that any further improvements would require a radically new method, instead of complicated inequalities with more terms.

Wu Dong Hua [53] claimed to have $C^* \leq 7.81565$, but some functions he defined to compute C^* failed to have some necessary properties [48].

[‡] Some authors instead include the factor of 2 inside C^*, so they instead assert $D(N) \sim \Theta(N)$ for (1.6), and $D(N) \leq 2C^*\Theta(N)$ for (1.8).

[†] We remind the reader than C^* is conjectured to be 2.

C^*	Year	Author
$16+\epsilon$	1949	Selberg [45]
12	1964	Pan [37]
8	1966	Bombieri & Davenport [3]
7.8342	1978	Chen [7]
7.8209	2004	Wu [54]

Table 1.1: Improvements of C^* in (1.8) over time, conjectured that $C^* = 2$.

1.5 The Linnik–Goldbach problem

The Linnik–Goldbach problem [41] is another weaker form of the GC, which asks for the smallest values of K such that for all sufficient large even N,

$$N = p_1 + p_2 + 2^{e_1} + 2^{e_2} + \ldots + 2^{e_r},\ r \leq K. \tag{1.9}$$

That is, we can express N as the sum of two primes and at most K powers of two (we refer to K as the Linnik–Goldbach constant). In 1953, Linnik [30] proved that there exists some finite K such that the statement holds, but did not include an explicit value for K. (See Table 1.2 for historical improvements on K.) The methods of Heath-Brown and Puchta [22], and of Pintz and Ruzsa [40] show that K satisfies (1.9) if

$$\lambda^{K-2} < \frac{C_3}{(C^*-2)C_2 + cC_0^{-1}\log 2},$$

for particular constants $\lambda, C_0, C^*, C_2, C_3, c$.

Here, C_0 is the twin primes constant, given by

$$C_0 = \prod_{\substack{p>2 \\ p \text{ prime}}} \left(1 - \frac{1}{(p-1)^2}\right) \approx 0.66016\ldots \tag{1.10}$$

The infinite product for C_0 is easily verified as convergent, as for all integers $n > 2$

$$0 < 1 - \frac{1}{(n-1)^2} < 1.$$

So C_0 is an infinite product, with each term strictly between 0 and 1. Therefore, $0 \leq C_0 < 1$. The value of C_0 is easily computed: Wrench provides C_0 truncated to 42 decimal places [52]. As far as lowering the value of K, improvements on the other constants will be required.

Now, C_2 is defined by

$$C_2 = \sum_{d=0}^{\infty} \left(\frac{|\mu(2d+1)|}{\epsilon(2d+1)} \prod_{\substack{p|d \\ p>2}} \frac{1}{p-2} \right),$$

where

$$\epsilon(n) = \min_{v \in \mathbb{N}} \{v : 2^v \equiv 1 \bmod d\}.$$

and $\mu(x)$ is the Möbius function. It has been shown by Khalfalah–Pintz [39] that

$$1.2783521041 < C_2 C_0 < 1.2784421041, \tag{1.11}$$

So since C_0 is easily computed, we can convert (1.11) to

$$1.93642 < C_2 < 1.93656. \tag{1.12}$$

It is remarked by Khalfalah–Pintz that estimating C_2 is very difficult, and that any further progress is unlikely. The remaining constants are defined by similarly complicated expressions (see [41]). Platt and Trudgian [41] make improvements on both C_3 and λ, by showing that one can take

$$(C_3, \lambda) = (3.02858417, 0.8594000)$$

and obtain unconditionally that $K \geq 11.0953$, a near miss for $K = 11$. Platt–Trudgian remark that any further improvements in estimating C_3 using their method with more computational power would be limited. Obtaining $K = 11$ by improving Chen's constant (assuming all others constants used by Platt–Trudgian are the same) would require $C^* \leq 7.73196$, which is close to the best known value of $C^* \leq 7.8209$. This provides a motivation for reducing C^*.

1.6 History of Romanov's constant

In 1849, de Polignac conjectured that every odd $n > 3$ can be written as a sum of an *odd* prime and a power of two. He found a counterexample $n = 959$, but an interesting question that follows is how many counterexamples are there? Are there infinitely many? If so, how common are they among the integers? If we let

$$A(N) = \#\{n : n < N, n = 2^m + p\} \tag{1.13}$$

K	K assuming GRH	Year	Author
-	$< \infty$	1951	Linnik [29]
$< \infty$	-	1953	Linnik [30]
54000	-	1998	Liu, Liu and Wang [31]
25000	-	2000	H.Z.Li [28]
-	200	1999	Liu, Liu and Wang [32]
2250	160	1999	T.Z.Wang [51]
1906	-	2001	H.Z.Li [27]
13	7	2002	Heath-Brown and Puchta* [22]
12	-	2011	Liu and Lü [33]

Table 1.2: Values of K in (1.9) over the years

$$R_- = \liminf_{N\to\infty} \frac{A(N)}{N} \quad R = \lim_{N\to\infty} \frac{A(N)}{N} \quad R_+ = \limsup_{N\to\infty} \frac{A(N)}{N}^{\dagger} \tag{1.14}$$

then R denotes the density of these decomposable numbers, and R_+ and R_- provide upper and lower bounds respectively.

Romanov [43] proved in 1934 that $R_- > 0$, though he did not provide an estimate on the value of R. An explicit lower bound on R was not shown until 2004, with Chen–Sun [8] who proved $R_- \geq 0.0868$. Habsieger–Roblot [18] improved both bounds, obtaining $0.0933 < R_- \leq R_+ < 0.49045$. Pintz [38] obtained $R_- \geq 0.09368$, but under the assumption of Wu Dong Hua's value of Chen's constant $C^* \leq 7.81565$, the proof of which is flawed [48].

Since $2n \neq p + 2^k$ for an odd prime p, it is trivial to show that $R_+ \leq 1/2$. Van de Corput [49] and Erdős [13] proved in 1950 that $R_+ < 0.5$. In 1983, Romani [42] computed $A(N)/N$ for all $N < 10^7$ and noted that the minima were located when N was a power of two. He then constructed an approximation to $A(N)$, by using an approximation to the prime counting function $\pi(x)$

$$\pi(x) \sim \mathrm{Li}(x) := \int_2^x \frac{1}{\log t}\, dt = \sum_{m=1}^{\infty} \frac{(m-1)!}{\log^m x} x,$$

then using the Taylor expansion of $\mathrm{Li}(x)$ to obtain a formula for $A(N)$ with

†Some authors denote $R = \lim_{n\to\infty} 2A(N)/N$ (and similar for R_+ and R_-), in which case the trivial bound is $R_+ \leq 1$.

*This was also proved independently by Pintz and Ruzsa [40] in 2003. They also claim to have $K \leq 8$, but this is yet to appear in literature.

unknown coefficients b_i

$$A(N) = Rx + \sum_{i=1}^{\infty} b_i \frac{x}{(\log x)^i}.$$

By using the precomputed values for $A(N)$, the unknown coefficients may be estimated, thus extrapolating values for $A(N)$. Using this method, Romani conjectured that $R \approx 0.434$.

Bomberi's [42] probabilistic approach, which randomly generates probable primes (as they are computationally faster to find than primes, and pseudoprimes[‡] are uncommon enough that it does not severely alter the results) in the interval $[1, n]$, in such a way that the distribution closely matches that of the primes, is also used to compute R. The values obtained closely match Romani's work, and so it is concluded that $R \approx 0.434$ is a reasonable estimate.

The lower bound to Romonov's constant R_-, the Linnik–Goldbach constant K and Chen's constant C^* are all related. There is a very complicated connection relating R_- and K [38], but here we prove a simple property relating R_- and K.

Proposition. *If $R_- > 1/4$, then $K \leq 2$ [38].*

Proof. If $R_- > 1/4$ then for any given even N, more than $1/4$ of the numbers up to N can be written as the sum of an odd prime and a power of two. No even n can be written as $n = p + 2^k$ since p is odd. So more than $1/2$ of the odd numbers up to N can be written in this way. If we construct a set of pairs of odd integers

$$\left\{(1, N-1), (3, N-3), \ldots, \left(\frac{N-r}{2}, \frac{N+r}{2}\right)\right\},$$

where $r = N \bmod 4$, then by the pigeon-hole principle, there must exist a pair $(k, N-k)$ such that

$$k = p_1 + 2^{v_1}, \quad N - k = p_2 + 2^{v_2}.$$

Therefore

$$N = k + (N-k) = p_1 + p_2 + 2^{v_1} + 2^{v_2}.$$ □

Pintz also proved the following theorems [38].

Theorem 1.6.1. *If $C^* = 2$ holds, then $R_- \geq 0.310987$.*

This can be combined with the proposition above to obtain a relationship between C^* and K, although Pintz also shows a weaker estimate on C^* is sufficient.

‡A composite number that a probabilistic primality test incorrectly asserts is prime.

Theorem 1.6.2. *If $C^* \leq 2.603226$, then $R_- > 1/4$ and consequently $K \leq 2$.*

As an explicit lower bound for R did not appear until 2004, and this bound is much lower than the expected 0.434 given by Romani, attempting to improve K by improving R_- appears a difficult task.

1.7 Chen's theorem

Chen's theorem [26] is another weaker form of Goldbach, which states that every sufficiently large even integer is the sum of two primes, or a prime and a semiprime (product of two primes). By letting $R(N)$ denotes the number of ways N can be decomposed in this manner, Chen attempts to get a lower bound on the number of ways N can be decomposed as $N = p + P_3$, where P_3 is some number with no more than three prime factors, using sieve theory methods. He then removes the representations where $N = p + p_1p_2p_3$ [19]. By doing so, Chen obtains that there exists some constant N_0 such that if N is even and $N > N_0$, then

$$\#\{p : p \leq N, n - p \in \mathbb{P}_2\} > 0.67\Theta(N),$$

where $\Theta(N)$ is the same function used for the conjectured tight bound of $D(N)$ (see 1.6). We have the asymptotic lower bound (see 1.7)

$$\Theta(N) \gg \frac{N}{\log^2 N}.$$

so this implies that for all sufficiently large even N

$$N = p + q \text{ for } q \in \mathbb{P}_2$$

In 2015, Yamada [55] proved that letting $N_0 = \exp\exp 36$ is sufficient for the above to hold.

Chapter 2

Preliminaries for Wu's paper

2.1 Summary

Wu [54] proved that $C^* \leq 7.8209$. He obtained this result by expressing the Goldbach conjecture as a linear sieve, and finding an upper bound on the size of the sieved set. The upper bound constructed is very complicated, using a series of weighted inequalities with 21(!) terms. The approximation to the sieve is computed using numerical integration, weighting the integrals over judicially chosen intervals. Few intervals (9), over which to discretise the integration are used, thereby reducing the problem to a linear optimisation with 9 equations.

> "If we divide the interval $[2, 3]$ into more than 9 subintervals, we can certainly obtain a better result. But the improvement is minuscule." [54, p. 253]

The main objective of this paper is to quantify how "minuscule" the improvement is.

2.2 Preliminaries of sieve theory

A sieve is an algorithm that takes a set of integers and *sifts out*, or removes, particular integers in the set based on some properties.

The classic example is the *Sieve of Eratosthenes* [21, Chpt 1], an algorithm devised by Erathosthenes in the 3rd century BC to generate all prime numbers below some bound. The algorithm proceeds as follows: Given the first n primes $\mathcal{P} = \{p_1, \ldots, p_n\}$, list the integers from 2 to $(p_n + 2)^2 - 1$. For each prime p in the set $\mathcal{P}$, strike out all multiples of p in the list starting from $2p$. All remaining numbers are primes below $(p_n+2)^2$, as the first number k that is composite and not struck out by this procedure must share no prime factors with $\mathcal{P}$. So $k = p_{n+1}^2 \geq (p_n+2)^2$.

This method of generating a large set of prime numbers is efficient, as by striking off the multiples of each prime from a list of numbers, the only operations used is addition and memory lookup. Contrast this with primality testing via trial division, as integer division is slower than integer addition. O'Neill [36] showed that to generate all primes up to a bound n, the Sieve of Eratosthenes takes $O(n \log\log n)$ operations whereas repeated trial division would take $O(n^{\frac{3}{2}}/\log^2 n)$ operations. Moreover, the Sieve of Eratosthenes does not use division in computing the primes, only addition.

Sieve theory is concerned with estimating the size of the sifted set. Formally, given a finite set $\mathcal{A} \subset \mathbb{N}$, a set of primes $\mathcal{P}$ and some number $z \geq 2$, we define the sieve function [21]

$$S(\mathcal{A}; \mathcal{P}, z) = \#\{a \in \mathcal{A} : \forall p \in \mathcal{P} \text{ with } p < z, (a,p) = 1\}, \tag{2.1}$$

i.e. by taking the set $\mathcal{A}$ and removing the elements that are divisible by some prime $p \in \mathcal{P}$ with $p < z$, the number of elements left over is $S(\mathcal{A}; \mathcal{P}, z)$. Removing the elements of $\mathcal{A}$ in this manner is called *sifting*. Analogous to a sieve that sorts through a collection of objects and only lets some through, the unsifted numbers are those in $\mathcal{A}$ that do not have a prime factor in $\mathcal{P}$. Many problems in number theory can be re-expressed as a sieve, and thus attacked. We provide an example related to the Goldbach conjecture included in [21]. For a given even N, let

$$\mathcal{A} = \{n(N-n) : n \in \mathbb{N}, 2 \leq n \leq N-2\}, \qquad \mathcal{P} = \mathbb{P}.$$

Then

$$S(\mathcal{A}, \mathbb{P}; \sqrt{N}) = \#\{n(N-n) : n \in \mathbb{N}, p < \sqrt{N} \Rightarrow (n(N-n), p) = 1\}.$$

Now since $(n(N-n), p) = 1 \Rightarrow (n,p) = 1$ and $(N-n, p) = 1$ for all $p < \sqrt{N}$, both n and $N-n$ must be prime, as if not, either n or $N-n$ has a prime factor $\geq \sqrt{N}$, which implies $n \geq N$ (impossible) or $N-n \geq N$ (also impossible). Hence

$$S(\mathcal{A}, \mathbb{P}; \sqrt{N}) = \#\{p \in \mathbb{P} : (N-p) \in \mathbb{P}, p < \sqrt{N}\},$$

Now for all primes p, if $p < \sqrt{N}$, then $p \leq N/2$, hence

$$\begin{aligned} S(\mathcal{A}, \mathbb{P}; \sqrt{N}) &\leq \#\{p \in \mathbb{P} : (N-p) \in \mathbb{P}, p \leq N/2\}, \\ &\leq \#\{p \in \mathbb{P} : (N-p) \in \mathbb{P}, p \leq N-p\} = D(N). \end{aligned}$$

So this particular choice of sieve is a lower bound for $D(N)$. If we have a particular (possibly infinite) subset of the integers $\mathcal{A}$, we may wish to take all numbers in $\mathcal{A}$ less that or equal to x, denoted* $\mathcal{A}_{\leq x}$

$$\mathcal{A}_{\leq x} = \{a \in \mathcal{A} : a \leq x\},$$

and ask how fast $\#\mathcal{A}_{\leq x}$ grows with x. For example, if $\mathcal{A}$ were the set of all even numbers,

$$\mathcal{A} = \{n \in \mathbb{N} : n \text{ even}\} = \{0, 2, 4, \ldots\},$$

the size of the set of $\mathcal{A}_{\leq x}$ would be computed as:

$$\#\mathcal{A}_{\leq x} = \#\{a \in \mathcal{A} : a \leq x\} = \left\lfloor \frac{x}{2} \right\rfloor + 1.$$

It is usually more difficult to figure out how sets grow. Likewise, an exact formula is usually impossible. Therefore, the best case is usually an asymptotic tight bound. For example, if $\mathcal{A} = \mathbb{P}$, the set of all primes, then the prime number theorem [1, p. 9] gives

$$\#\{p \in \mathbb{P} : p \leq n\} = \pi(x) \sim \frac{x}{\log x}.$$

The main aim of sieve theory is to decompose $\#\mathcal{A}_{\leq N}$ as the sum of a main term X and an error term R, such that X dominates R for large N. We can then obtain an asymptotic formula for $\#\mathcal{A}_{\leq N}$ [19]. This partially accounts for the many proofs in number theory that only work for some extremely large N, where N can be gargantuan (see the Ternary Goldbach conjecture in Chapter 1), as the main term may only dominate the error term for very large values. In some cases it can only be shown that the main term eventually dominates the error term, no explicit value as to how large N needs to be before this occurs is required.

Now, for a given subset $\mathcal{A}_{\leq x}$, we choose a main term† X that is hopefully a good approximation of $\#\mathcal{A}_{\leq x}$.

We denote

$$\mathcal{A}_d = \{a : a \in \mathcal{A}_{\leq x}, a \equiv 0 \bmod d\},$$

for some square-free number d. For each prime p, we assign a value for the function $\omega(p)$, with the constraint that $0 \leq \omega(p) < p$, so that

$$\#\mathcal{A}_p \approx \frac{\omega(p)}{p} X.$$

*In the literature, it is common to use $\mathcal{A}$ instead of $\mathcal{A}_{\leq x}$, and it is implicitly understood that $\mathcal{A}$ only includes the numbers less than some x.

†Note that since X depends on x, we would normally write $X(x)$, but we wished to stick to convention.

By defining

$$\omega(1) = 1, \quad \omega(d) = \prod_{p|d} \omega(p),$$

for all square-free d, we ensure that $\omega(d)$ is a multiplicative function. We now define the error term (sometimes called the remainder term):

$$R_d = \#\mathcal{A}_d - \frac{\omega(d)}{d} X.$$

So we have that

$$\#\mathcal{A}_d = \frac{\omega(d)}{d} X + R_d,$$

where (hopefully) the main term $\frac{\omega(d)}{d}X$ dominates the error term R_d. Given a set of prime numbers $\mathcal{P}$, we define

$$P(z) = \prod_{p \in \mathcal{P}, p < z} p.$$

We can rewrite the sieve using two identities of the Möbius function and multiplicative functions.

Theorem 2.2.1. *[1, Thm 2.1] If* $n \geq 1$ *then*

$$\sum_{d|n} \mu(d) = \begin{cases} 1 & n = 1, \\ 0 & n > 1. \end{cases} \tag{2.2}$$

Proof. The case $n = 1$ is trivial. For $n > 1$, write the prime decomposition of n as $n = p_1^{e_1} \dots p_n^{e_n}$. Since $\mu(d) = 0$ when d is divisible by a square, we need only consider divisors d of n of the form $d = p_1^{a_1} \dots p_n^{a_n}$, where each a_i is either zero or one, (i.e., divisors that are products of distinct primes). Enumerating all possible products made from $\{p_1, \dots, p_n\}$, we obtain

$$\begin{aligned} \sum_{d|n} \mu(d) &= \mu(1) + \Big(\mu(p_1) + \ldots + \mu(p_n)\Big) + \Big(\mu(p_1 p_2) \\ &\quad + \ldots + \mu(p_{n-1} p_n)\Big) + \ldots + \mu(p_1 \ldots p_n) \\ &= 1 + \binom{n}{1}(-1) + \binom{n}{2}(1) + \ldots + \binom{n}{n}(-1)^n \\ &= \sum_{i=0}^{n} \binom{n}{i}(-1)^i = (1-1)^n = 0. \end{aligned}$$

□

Theorem 2.2.2. *[1, Thm 2.18] If f is multiplicative* [‡] *we have*

$$\sum_{d|n} \mu(d) f(d) = \prod_{p|n} (1 - f(p)). \tag{2.3}$$

Proof. Let

$$g(n) = \sum_{d|n} \mu(d) f(d).$$

Then $g(n)$ is multiplicative, as

$$\begin{aligned} g(pq) &= \sum_{d|pq} \mu(d) f(d) = \mu(1) f(1) + \mu(p) f(p) + \mu(q) f(q) + \mu(pq) f(pq), \\ &= 1 - f(p) - f(q) + f(p) f(q) = (1 - f(p))(1 - f(q)), \\ &= \left(\sum_{d|p} \mu(d) f(d) \right) \left(\sum_{d|q} \mu(d) f(d) \right) = g(p) g(q). \end{aligned}$$

So by letting $n = p_1^{a_1} \dots p_n^{a_n}$, we have

$$g(n) = \prod_{i=1}^{n} g(p_i^{a_i}) = \prod_{i=1}^{n} \sum_{d|p_i^{a_i}} \mu(d) f(d).$$

Now since $\mu(d)$ is zero for $d = p^2, p^3, \dots$, the only non-zero terms that are divisors of $p_i^{a_i}$ are 1 and p_i.

$$g(n) = \prod_{i=1}^{n} (\mu(1) f(1) + \mu(p_i) f(p_i)) = \prod_{i=1}^{n} (1 - f(p_i)) = \prod_{p|n} (1 - f(p)).$$

□

Now given this, we can rewrite the sieve as

$$\mathcal{S}(\mathcal{A}, \mathcal{P}, x) = \sum_{\substack{n \in \mathcal{A} \\ (n, P(z)) = 1}} 1 = \sum_{n \in \mathcal{A}} \sum_{\substack{d|n \\ d|P(z)}} \mu(d) = \sum_{d|P(z)} \mu(d) \# \mathcal{A}_d, \tag{2.4}$$

as we sum over all $n \in \mathcal{A}$ such that a is square-free, as the Möbius function is only non-zero for square-free inputs. Using the approximation to $\#\mathcal{A}_d$, we obtain

$$\begin{aligned} \mathcal{S}(\mathcal{A}, \mathcal{P}, x) &= X \sum_{d|P(z)} \frac{\mu(d) \omega(d)}{d} + \sum_{d|P(z)} \mu(d) R_d, \\ &= X \prod_{p|P(z)} \left(1 - \frac{\omega(p)}{p} \right) + \sum_{d|P(z)} \mu(d) R_d. \end{aligned} \tag{2.5}$$

[‡]A function f is multiplicative if $f(m)f(n) = f(mn)$ whenever $\gcd(n, m) = 1$.

Writing

$$W(z;\omega) = \prod_{p<z, p\in\mathcal{P}} \left(1 - \frac{\omega(p)}{p}\right),$$

we obtain

$$|S(\mathcal{A};\mathcal{P},z) - XW(z;\omega)| \leq \left|\sum_{d|P(z)} \mu(d)R_d\right|.$$

Then, by using the triangle inequality, we obtain the worst case remainder when all the $\mu(d)$ terms in the sum are one

$$|S(\mathcal{A};\mathcal{P},z) - XW(z;\omega)| \leq \sum_{d|P(z)} |R_d|. \tag{2.6}$$

This is the Sieve of Eratosthenes–Legendre, which crudely bounds the error between the actual sieved set and the approximations generated by choosing X and $\omega(p)$. Sometimes, even approximating this sieve proves too difficult, so the problem is weakened before searching for an upper or lower bound. For example, see (1.7). For an upper bound, we search for functions $\mu^+(d)$ that act as upper bounds to $\mu(d)$, in the sense that

$$\sum_{d|(n,P(z))} \mu^+(d) \geq \sum_{d|(n,P(z))} \mu(d) = \begin{cases} 1 & (n,P(z)) = 1, \\ 0 & (n,P(z)) > 1. \end{cases} \tag{2.7}$$

Then

$$S(\mathcal{A};\mathcal{P},z) \leq X \sum_{d|P(z)} \frac{\mu^+(d)\omega(d)}{d} + \sum_{d|P(z)} |\mu^+(d)||R_d|. \tag{2.8}$$

Minimising the upper bound while ensuring $\mu^+(d)$ satisfies (2.7) and has sufficiently small support (to reduce the size of the summation) is, in general, very difficult. Nevertheless, this method is used by Chen [26] to construct the following upper bounds of sieves that we have related to the Goldbach conjecture and the twin primes conjecture [§].

$$\#\{(p,p') : p \in \mathbb{P}, p' \in \mathbb{P}_{\leq 2}, p + p' = 2n\} \gg \frac{n}{\log^2 n} \tag{2.9}$$

$$\#\{p \in \mathbb{P} : p \leq x, p+2 \in \mathbb{P}_{\leq 2}\} \gg \frac{x}{\log^2 x} \tag{2.10}$$

where $\mathbb{P}_{\leq 2}$ is the set of all integers with 1 or 2 prime factors.

[§] The twin primes conjecture asserts the existence of infinitely many primes p for which $p+2$ is also prime. Examples include 3 and 5, 11 and 13, 41 and 43, ...

The first sieve is a near miss for approximating the Goldbach sieve, and weakens the Goldbach conjecture to allow sums of primes, or a prime and a semiprime¶. The second sieve similarly weakens the twin primes conjecture. Thus, Chen's sieves imply that there are infinitely many primes p such that $p+2$ is either prime or semiprime, and that every sufficiently large even integer n can be decomposed into the sum of a prime and a semiprime. However, the asymptotic bounds above do not show constants that may be present, so "sufficiently large" could be very large indeed.

2.3 Selberg sieve

Let $\lambda_1 = 1$ and for $d \geq 2$, let $\lambda_d \geq 2$ be arbitrary real numbers. By (2.4), we can construct the upper bound

$$\mathcal{S}(\mathcal{A},\mathcal{P},z) = \sum_{n\in\mathcal{A}} \sum_{\substack{d\mid n \\ d\mid P(z)}} \mu(d) \leq \sum_{n\in\mathcal{A}} \left(\sum_{\substack{d\mid n \\ d\mid P(z)}} \lambda_d \right)^2 . \tag{2.11}$$

By squaring and rearranging the order of summations [19], we obtain

$$\mathcal{S}(\mathcal{A},\mathcal{P},z) \leq \sum_{\substack{d_v\mid P(z) \\ v=1,2}} \lambda_{d_1}\lambda_{d_2} \sum_{\substack{a\in\mathcal{A} \\ a\equiv 0 \bmod \operatorname{lcm}(d_1,d_2)}} 1. \tag{2.12}$$

This is used to construct an upper bound for the sieve in the same form as (2.8).

$$S(\mathcal{A};\mathcal{P},z) \leq X \sum_{\substack{d_v\mid P(z) \\ v=1,2}} \lambda_{d_1}\lambda_{d_2}\frac{\omega(D)}{D} + \sum_{\substack{d_v\mid P(z) \\ v=1,2}} |\lambda_{d_1}\lambda_{d_2}R_D| = X\Sigma_1 + \Sigma_2, \tag{2.13}$$

Now one can choose the other remaining constants $\lambda_d, d \geq 2$ so that the main term Σ_1 is as small an upper bound as possible, while ensuring Σ_1 dominates Σ_2. Since this is in general very difficult even for simple sequences $\mathcal{A}$, Selberg looked at the more restricted case of setting all the constants

$$\lambda_d = 0 \text{ for } d \geq z$$

and then choosing the remaining λ_d terms to minimise Σ_1, which is now a quadratic in λ_d. Having fewer terms to deal with makes it easier to control, and hence to bound the size of the remainder term Σ_2.

¶A semiprime is a product of two primes.

Chapter 3

Examining Wu's paper

In this chapter we look at the section of Wu's paper needed to compute C^*.

3.1 Chen's method

Chen wished to take the set

$$\mathcal{A} = \{N - p : p \le N\},$$

and apply a sieve to it, keeping only the integers in $\mathcal{A}$ that are prime. This leaves the set of all primes of the form $N - p$, which (due to double counting) is asymptotic to $2D(N)$.

The goal is to approximate the sieve $S(\mathcal{A}; \mathcal{P}, z)$, as described in Chapter 2. Chen uses the sieve Selberg [45] used to prove $C^* \le 16 + \epsilon$, which has some extra constraints on the multiplicative function $\omega(p)$ in the main term, to make it easier to estimate. Define

$$V(z) = \prod_{p<z} \left(1 - \frac{\omega(p)}{p}\right) \tag{3.1}$$

and suppose there exists a constant $K > 1$ such that

$$\frac{V(z_1)}{V(z_2)} \le \frac{\log z_2}{\log z_1} \left(1 + \frac{K}{\log z_1}\right) \text{ for } z_2 \ge z_1 \ge 2. \tag{3.2}$$

Then the Rosser–Iwaniec [25] linear sieve is given by

$$S(\mathcal{A}; \mathcal{P}, z) \le XV(z) \left\{ F\left(\frac{\log Q}{\log z}\right) + E \right\} + \sum_{l<L} \sum_{q|P(z)} \lambda_l^+(q) r(\mathcal{A}, q), \tag{3.3}$$

$$S(\mathcal{A}; \mathcal{P}, z) \ge XV(z) \left\{ f\left(\frac{\log Q}{\log z}\right) + E \right\} - \sum_{l<L} \sum_{q|P(z)} \lambda_l^-(q) r(\mathcal{A}, q), \tag{3.4}$$

where F and f are the solutions of the following coupled difference equations, *

$$F(u) = 2e^{-\gamma}/u, \qquad f(u) = 0, \qquad (0 < u \le 2) \tag{3.5}$$
$$(uF(u))' = f(u-1), \qquad (uf(u))' = F(u-1), \qquad (u \ge 2) \tag{3.6}$$

The Rosser–Iwaniec sieve is a more refined version of Selbergs sieve, as the error terms λ_l^+ and λ_l^- have some restrictions that, informally, λ_l^+ (or λ_l^-) can be decomposed into the convolution of two other functions $\lambda = \lambda_1 * \lambda_2$. We will be concerned only with (3.3), as we only need to find an upper bound for the sieve. Lower bounds on the sieve would imply the Goldbach conjecture, which would be difficult. Chen improved on the sieve (3.3) by introducing two new functions $H(s)$ and $h(s)$ such that (3.3) holds with $f(s) + h(s)$ and $F(s) - H(s)$ in place of $f(s)$ and $F(s)$ respectively.[54].

$$S(\mathcal{A}; \mathcal{P}, z) \le XV(z)\left\{(F(s) - H(s))\left(\frac{\log Q}{\log z}\right) + E\right\} + \text{error}, \tag{3.7}$$

Chen proved that $h(s) > 0$ and $H(s) > 0$ (which is obviously a required property, as otherwise these functions would make the bound on $S(\mathcal{A}; \mathcal{P}, z)$ worse) using three set of complicated inequalities (the largest had 43 terms!).

3.2 Wu's improvement

Wu followed the same line of reasoning as Chen, but created a new set of inequalities that describe the functions $H(s)$ and $h(s)$. Wu's inequalities are both simpler (having only 21 terms) and make for a tighter bound on $S(\mathcal{A}; \mathcal{P}, z)$. We will not look into the inequalities, but rather a general overview of the method Wu used. For full details, see [54, p. 233].

Let $\delta > 0$ be a sufficiently small number, $k \in \mathbb{N}$ and $0 \le i \le k$. Define

$$Q = N^{1/2-\delta}, \quad \underline{d} = Q/d, \quad \mathcal{L} = \log N, \quad W_k = N^{d^{1+k}}. \tag{3.8}$$

Let $\Delta \in \mathbb{R}$ such that $1 + \mathcal{L}^{-4} \le \Delta \le 1 + 2\mathcal{L}^{-4}$.

Define

$$A(s) = sF(s)/2e^{-\gamma}, \quad a(s) = sf(s)/2e^{\gamma}, \tag{3.9}$$

where F and f are defined by (3.5) and (3.6).

*The astute reader will note the similarity between F, f and the Buchstab function $\omega(u)$ (see 4.1)

Define

$$\Phi(N, \sigma, s) = \sum_{d} \sigma(d)\mathcal{S}(\mathcal{A}_d, \{p : (p, dN) = 1\}, \underline{d}^{1/s}), \tag{3.10}$$

where σ is a arithmetical function that is the Dirchlet convolution of a collection of characteristic functions

$$\sigma = \mathbf{1}_{E_1} * \ldots * \mathbf{1}_{E_i},$$

where

$$E_j = \{p : (p, N) = 1\} \cap [V_j/\Delta, V_j),$$

and $V_1, \ldots, V_i$ are real numbers satisfying a set of inequalities[54, p. 244]. Informally, the inequalities state that the V_i terms are ordered in size, bounded below by W_k

$$V_1 \geq \ldots \geq V_i \geq W_k,$$

and that no one V_i term can be too large. Each V_i term is bounded above by both Q and the previous terms $V_1, \ldots, V_{i-1}$.

$$V_i \leq \sqrt{\frac{Q}{V_1 \ldots V_{i-1}}}.$$

So if any one V_i term is big, the rest of the terms beyond will be constrained to be small.

Φ can be thought of as breaking up the sieve $S(\mathcal{A}; \mathcal{P}, z)$ into smaller parts, where the set that is being sieved over is only those elements in $\mathcal{A}$ that are multiples of d, and the index of summation is given by the σ, as $\sigma(d)$ will be zero everywhere expect on its set of support. Beaking up the sieve this was allows Wu to prove some weighted inequalities reated to Φ, that would ordinarily be too difficult to prove in general for the entire sieve.

Define

$$\Theta(N, \sigma) = 4\text{Li}(N) \sum_{d} \frac{\sigma(d) C_{dN}}{\varphi(d) \log \underline{d}}, \tag{3.11}$$

where C_N is defined in (1.6).

Now for $k \in \mathbb{N}^+, N_0 \geq 2$ and $s \in [1, 10]$ we defined $H_{k,N_0}(s)$ and h_{k,N_0} as the supremum of h such that for all $N \geq N_0$ and functions σ comprised of the convolution of no more than k characteristic functions, the following inequalities hold

$$\Phi(N, \sigma, s) \leq \{A(s) - h\}\Theta(N, \sigma), \qquad \Phi(N, \sigma, s) \geq \{a(s) + h\}\Theta(N, \sigma). \tag{3.12}$$

Wu shows that both $H_{k,N_0}(s)$ and h_{k,N_0} are decreasing, and defines

$$H(s) = \lim_{k\to\infty}\left(\lim_{N_0\to\infty} H_{k,N_0}(s)\right), \qquad h(s) = \lim_{k\to\infty}\left(\lim_{N_0\to\infty} h_{k,N_0}(s)\right) \tag{3.13}$$

Now it is very difficult to get an explicit form of H or h, or to even conclude anything about the behaviour beyond it is decreasing. Wu proceeds by proving the following integral equations

$$h(s) \geq h(s') + \int_{s-1}^{s'-1} \frac{H(t)}{t}dt, \quad H(s) \geq H(s') + \int_{s-1}^{s'-1} \frac{h(t)}{t}dt, \tag{3.14}$$

These integral equations are still difficult to work with, as all Wu proves about h and H is that $H(s)$ is decreasing on $[1, 10]$, and $h(s)$ is increasing on $[1, 2]$, and is decreasing on $[2, 10]$.

Wu proves an upper bound for the smaller parts of the sieve Φ

$$5\Phi(N, \sigma, s) \leq \sum_d \sigma(d)(\Gamma_1 - \ldots - \Gamma_4 + \Gamma_5 + \ldots + \Gamma_{21}) + O_{\delta,k}(N^{1-\eta})$$
$$2\Phi(N, \sigma, s) \leq \sum_d \sigma(d)(\Omega_1 - \Omega_2 + \Omega_3) + O_{\delta,k}(N^{1-\eta})$$

where the Γ_i terms are the dreaded 21 terms in Wu's weighted inequality [54, p.233]. Wu uses this weighted inequality

3.3 A lower bound for $H(s)$

Now to get an upper bound on the sieve, Wu needs to compute $H(s)$. The integral equation is difficult to resolve, so it is weakened to give a lower bound for $H(s)$, given the following Wu obtains two lower bounds for $H(s)$,

Proposition 3.3.1. *For $2 \leq s \leq 3 \leq s' \leq 5$ and $s' - s'/s \geq 2$, we have*

$$H(s) \geq \Psi_1(s) + \int_1^3 H(t)\Xi_1(t, s)\, dt, \tag{3.15}$$

where $\Xi(t, s) = \Xi(t, s, s')$ is given by

$$\begin{aligned}\Xi_1(t, s, s') :=& \frac{\sigma_0(t)}{2t}\log\left(\frac{16}{(s-1)(s'-1)}\right) + \frac{\mathbf{1}_{[\alpha_2,3]}(t)}{2t}\log\left(\frac{(t+1)^2}{(s-1)(s'-1)}\right)\\ &+ \frac{\mathbf{1}_{[\alpha_3,\alpha_2]}(t)}{2t}\log\left(\frac{t+1}{(s-1)(s'-1-t)}\right),\end{aligned} \tag{3.16}$$

and where $\Psi(s) = \Psi(s, s')$ *is given by*

$$\Psi_1(s, s') := \int_2^{s'-1} \frac{\log(t-1)}{t} dt + \frac{1}{2} \int_{1-1/s}^{1-1/s'} \frac{\log(s't-1)}{t(1-t)} dt - I_1(s, s'), \tag{3.17}$$

where $I_1(s, s')$ *is defined as*

$$I_1(s, s') = \max_{\phi \geq 2} \iiint\limits_{1/s' \leq t \leq u \leq v \leq 1/s} \omega\left(\frac{\phi - t - u - v}{u}\right) \frac{dt\, du\, dv}{tu^2 v}, \tag{3.18}$$

and $\omega(u)$ *is the Buchstab Function, see (4.1).*

The equations $\Xi(s)$ and $\Psi_1(s)$ are derived from Wu's sieve inequalities, and they provide a way to rewrite the complicated integral equations (3.14) into an inequality that can be attacked.

Proposition 3.3.2. *For* $2 \leq s \leq 3 \leq s' \leq 5$ *and* $s \leq k_3 \leq k_2 \leq k_1 \leq s'$ *such that*

$$s' - s'/s \geq 2, \qquad 1 \leq \alpha_i \leq 3 \text{ for } (1 \leq i \leq 9), \qquad \alpha_1 < \alpha_4, \qquad \alpha_5 < \alpha_8$$

are all satisfied, then

$$H(s) \geq \Psi_2(s) + \int_1^3 H(s)\Xi_2(t, s)\, dt, \tag{3.19}$$

where $\Psi_2(s) = \Psi_2(s, s', k_1, k_2, k_3)$ is given by

$$\begin{aligned}\Psi_2(s, s', k_1, k_2, k_3) = &-\frac{2}{5}\int_2^{s'-1} \frac{\log(t-1)}{t}\, dt - \frac{2}{5}\int_2^{k_1-1} \frac{\log(t-1)}{t}\, dt \\ &-\frac{1}{5}\int_2^{k_2-1} \frac{\log(t-1)}{t}\, dt + \frac{1}{5}\int_{1-1/s}^{1-1/s'} \frac{\log(s't-1)}{t(1-t)}\, dt \\ &+\frac{1}{5}\int_{1-1/k_3}^{1-1/k_1} \frac{\log(k_1 t-1)}{t(1-t)}\, dt - \frac{2}{5}\sum_{i=9}^{25} I_{2,i}(s).\end{aligned} \tag{3.20}$$

and where $I_{2,i}(s) = I_{2,i}(s, s', k_1, k_2, k_3)$ is given by

$$
\begin{aligned}
I_{2,i}(s) &= \max_{\phi\geq 2} \int\limits_{\mathbb{D}_{2,i}} \omega\left(\frac{\phi-t-u-v}{u}\right)\frac{dt\,du\,dv}{tu^2v} \qquad (9\leq i\leq 15),\\
I_{2,i}(s) &= \max_{\phi\geq 2} \int\limits_{\mathbb{D}_{2,i}} \omega\left(\frac{\phi-t-u-v-w}{v}\right)\frac{dt\,du\,dv\,dw}{tuv^2w} \qquad (16\leq i\leq 19),\\
I_{2,20}(s) &= \max_{\phi\geq 2} \int\limits_{\mathbb{D}_{2,20}} \omega\left(\frac{\phi-t-u-v-w-x}{w}\right)\frac{dt\,du\,dv\,dw\,dx}{tuv^2x},\\
I_{2,21}(s) &= \max_{\phi\geq 2} \int\limits_{\mathbb{D}_{2,21}} \omega\left(\frac{\phi-t-u-v-w-x-y}{x}\right)\frac{dt\,du\,dv\,dw\,dx\,dy}{tuvwx^2y}.
\end{aligned} \tag{3.21}
$$

and the domains of integration are

$$
\begin{aligned}
\mathbb{D}_{2,9} &= \{(t,u,v) : 1/k_1 \leq t \leq u \leq v \leq 1/k_3\},\\
\mathbb{D}_{2,10} &= \{(t,u,v) : 1/k_1 \leq t \leq u \leq 1/k_2 \leq v \leq 1/s\},\\
\mathbb{D}_{2,11} &= \{(t,u,v) : 1/k_1 \leq t \leq 1/k_2 \leq u \leq v \leq 1/k_3\},\\
\mathbb{D}_{2,12} &= \{(t,u,v) : 1/s' \leq t \leq u \leq 1/k_1, 1/k_3 \leq v \leq 1/s\},\\
\mathbb{D}_{2,13} &= \{(t,u,v) : 1/s' \leq t \leq 1/k_1 \leq u \leq 1/k_2 \leq v \leq 1/s\},\\
\mathbb{D}_{2,14} &= \{(t,u,v) : 1/s' \leq t \leq 1/k_1, 1/k_2 \leq u \leq v \leq 1/s\},\\
\mathbb{D}_{2,15} &= \{(t,u,v) : 1/k_1 \leq t \leq 1/k_2 \leq u \leq 1/k_3 \leq v \leq 1/s\},\\
\mathbb{D}_{2,16} &= \{(t,u,v,w) : 1/k_2 \leq t \leq u \leq v \leq w \leq 1/k_3\},\\
\mathbb{D}_{2,17} &= \{(t,u,v,w) : 1/k_2 \leq t \leq u \leq v \leq 1/k_3 \leq w \leq 1/s\},\\
\mathbb{D}_{2,18} &= \{(t,u,v,w) : 1/k_2 \leq t \leq u \leq 1/k_3 \leq v \leq w \leq 1/s\},\\
\mathbb{D}_{2,19} &= \{(t,u,v,w) : 1/k_1 \leq t \leq 1/k_2, 1/k_3 \leq u \leq v \leq w \leq 1/s\},\\
\mathbb{D}_{2,20} &= \{(t,u,v,w,x) : 1/k_2 \leq t \leq 1/k_3 \leq u \leq v \leq w \leq x \leq 1/s\},\\
\mathbb{D}_{2,21} &= \{(t,u,v,w,x,y) : 1/k_3 \leq t \leq u \leq v \leq w \leq x \leq y \leq 1/s\}.
\end{aligned} \tag{3.22}
$$

This large set of integrals is derived by finding an integral equation that provides an upper bound for each term of the form

$$\sum_d \sigma(d)\Gamma_i$$

Taking the sum of all these integrals will give a bound for Φ, and hence for $H(s)$.

The α_i terms are given by

$$\alpha_1 := k_1 - 2, \qquad \alpha_2 := s' - 2,$$
$$\alpha_3 := s' - s'/s - 1, \qquad \alpha_4 := s' - s'/k_2 - 1,$$
$$\alpha_5 := s' - s'/k_3 - 1, \qquad \alpha_6 := s' - 2s'/k_2,$$
$$\alpha_7 := s' - s'/k_1 - s'/k_3, \qquad \alpha_8 := s' - s'/k_1 - s'/k_2$$
$$\alpha_9 := k_1 - k_1/k_2 - 1.$$

The function $\Xi_2(t,s) = \Xi_2(t,s,s',k_1,k_2,k_3)$ is given by

$$\begin{aligned}
\Xi_2(t;s) := \frac{\sigma_0(t)}{5t} \log\left(\frac{1024}{(s-1)(s'-1)(k_1-1)(k_2-1)(k_3-1)}\right) \\
+ \frac{\mathbf{1}_{[\alpha_2,3]}(t)}{5t} \log\left(\frac{(t+1)^5}{(s-1)(s'-1)(k_1-1)(k_2-1)(k_3-1)}\right) \\
+ \frac{\mathbf{1}_{[\alpha_9,\alpha_1]}(t)}{5t} \log\left(\frac{t+1}{(k_2-1)(k_1-1-t)}\right) \\
+ \frac{\mathbf{1}_{[\alpha_5,\alpha_2]}(t)}{5t} \log\left(\frac{t+1}{(k_3-1)(s'-1-t)}\right) \\
+ \frac{\mathbf{1}_{[\alpha_3,\alpha_2]}(t)}{5t} \log\left(\frac{t+1}{(s-1)(s'-1-t)}\right) \\
+ \frac{\mathbf{1}_{[\alpha_1,\alpha_2]}(t)}{5t} \log\left(\frac{(t+1)^2}{(k_1-1)(k_2-1)}\right) \\
+ \frac{\mathbf{1}_{[\alpha_7,\alpha_5]}(t)}{5t(1+t/s')} \log\left(\frac{s'^2}{(k_1s'-s'-k_1t)(k_3s'-s'-k_3t)}\right) \\
+ \frac{\mathbf{1}_{[\alpha_5,\alpha_8]}(t)}{5t(1-t/s')} \log\left(\frac{s'(s'-1-t)}{k_1s'-s'-k_1t}\right) \\
+ \frac{\mathbf{1}_{[\alpha_6,\alpha_8]}(t)}{5t(1-t/s')} \log\left(\frac{s'}{k_2s'-s'-k_2t}\right) \\
+ \frac{\mathbf{1}_{[\alpha_8,\alpha_2]}(t)}{5t(1-t/s')} \log\left(s'-1-t\right).
\end{aligned} \tag{3.23}$$

Ξ_2, together with the α terms, are derived by a complicated Lemma [54, p. 248] relating three separate integral inequality equations.

where

$$\sigma(a,b,c) := \int_a^b \log\frac{c}{t-1}\frac{1}{t}\,dt, \qquad \sigma_0(t) := \frac{\sigma(3,t+2,t+1)}{1-\sigma(3,5,4)}. \tag{3.24}$$

where

All of these complicated integrals are a way of bounding Wu's 21 term inequality. For each term Γ_i in the inequality, it has a corresponding integral. For example, here is one term from the inequality,

$$\Gamma_{10} = \sum_{\underline{d}^{1/k_1} \leq p_1 \leq p_2 \leq \underline{d}^{1/k_2} \leq p_3 \leq \underline{d}^{1/s}} \sum \sum \mathcal{S}(\mathcal{A}_{dp_1p_2p_3}, \{p : (p, dN) = 1\}, p_2\}) \tag{3.25}$$

which corresponds to

$$I_{2,10}(s) = \max_{\phi \geq 2} \int_{1/k_1 \leq t \leq u \leq 1/k_2 \leq v \leq 1/s} \omega\left(\frac{\phi - t - u - v}{u}\right) \frac{dt\, du\, dv}{tu^2 v}$$

The sieve is related to the function F, as F is part of the upper bound for the sieve (3.7). Now if we define the Dickman function $\rho(u)$ by

$$\begin{aligned} \rho(u) &= 1 & 1 \leq u \leq 2, \\ (u-1)\rho'(u) &= -\rho(u-1) & u \geq 2. \end{aligned} \tag{3.26}$$

then we can actually write F and f in terms of ω and ρ [19].

$$F(u) = e^{\gamma}\left(\omega(u) + \frac{\rho(u)}{u}\right), u > 0, \tag{3.27}$$

$$f(u) = e^{\gamma}\left(\omega(u) - \frac{\rho(u)}{u}\right), u > 0. \tag{3.28}$$

which provides a way to link the Buchstab function back to the sieve.

3.4 Discretising the integral

Wu comments that obtaining an exact solution is very difficult, and provides a lower bound on $H(s)$ by splitting up the integrals in 3.15 and 3.19 into 9 pieces. By letting $s_0 := 1$ and $s_i := 2.1 + 0.1i$ for $i = 1, \ldots, 9$, and the fact that $H(s)$ is decreasing on the interval $[1, 10]$, Wu obtains

$$H(s_i) \geq \Psi_2(s_i) + \sum_{j=1}^{9} a_{i,j} H(s_j) \tag{3.29}$$

where

$$a_{i,j} := \int_{s_{j-1}}^{s_j} \Xi_2(t, s_i) dt \quad i = 1, \ldots, 4;\ j = 1, \ldots, 9$$

and

$$H(s_i) \geq \Psi_1(s_i) + \sum_{j=1}^{9} a_{i,j} H(s_j) \tag{3.30}$$

where

$$a_{i,j} := \int_{s_{j-1}}^{s_j} \Xi_1(t, s_i)dt \quad i = 5, \dots, 9;\ j = 1, \dots, 9$$

Now $H(s_i)$ is given as a linear combination of all the other $H(s_j), 1 \leq j \leq 9$ values, which simplifies the problem from resolving a complicated integral equation, to a simple linear optimisation problem. These discretisations of the integrals can be written as matrix equations.

$$\mathbf{A} := \begin{bmatrix} a_{1,1} & \dots & a_{1,9} \\ \vdots & \ddots & \vdots \\ a_{9,1} & \dots & a_{9,9} \end{bmatrix}, \quad \mathbf{H} := \begin{bmatrix} H(s_1) \\ \vdots \\ H(s_9) \end{bmatrix}, \quad \mathbf{B} := \begin{bmatrix} \Psi_2(s_1) \\ \vdots \\ \Psi_2(s_4) \\ \Psi_1(s_5) \\ \vdots \\ \Psi_1(s_9) \end{bmatrix} \tag{3.31}$$

Thus 3.29 and 3.30 can be rewritten as

$$(\mathbf{I} - \mathbf{A})\mathbf{H} \geq \mathbf{B} \tag{3.32}$$

Wu further simplifies the problem by simply changing the inequality to an equality, and solves the system of simultaneous linear equations. This provides a lower bound to the linear optimisation problem given. So the equation below is solved for $\mathbf{X}$, which is easy to do.

$$(\mathbf{I} - \mathbf{A})\mathbf{X} = \mathbf{B} \tag{3.33}$$

Thus, we obtain that

$$\mathbf{H} \geq \mathbf{X} \tag{3.34}$$

Chen's constant is then equal to the largest element in the vector $\mathbf{X}$, as that corresponds to a lower bound for $H(s)$ at some point s. Bounds on H give us bounds on the sieve, by (3.7). Naturally, we choose the best element in $\mathbf{X}$ (i.e. the largest) to get the best bound on $\mathbf{H}$. It happens to be that the first element in $\mathbf{X}$ is always the biggest, as the function $\Psi_2(s)$ is maximised at approximately $s = 2.2$. Now, by taking $\sigma = \{1\}$ and $s = 2.2$ in the sum of sieves $\Phi(N, \sigma, s)$ (3.10)

$$\begin{aligned} \Phi(N, \{1\}, 2.2) &= \sum_d \sigma(d)\mathcal{S}(\mathcal{A}_d, \{p : (p, dN) = 1\}, \underline{d}^{1/2.2}), \\ &= \mathcal{S}(\mathcal{A}, \{p : (p, N) = 1\}, \underline{d}^{1/2.2}), \\ &= \mathcal{S}(\mathcal{A}, \{p : (p, N) = 1\}, N^{(1/2-\delta)/2.2}), \end{aligned}$$

By letting

$$A(s) = sF(s)/2e^{\gamma}$$

and from the definition of $\Theta(N, \sigma)$,

$$\begin{aligned}\Theta(N, \{1\}) &= 4\text{Li}(N) \sum_{d} \frac{C_N}{\log \underline{d}} \\ &= \frac{4\text{Li}(N) C_N}{\log N^{1/2-\delta}}\end{aligned}$$

Therefore, [54, p. 253]

$$\Phi(N, \{1\}, 2.2) \leq \{A(2.2) - H_{k,N_0}(2.2)\} \frac{4\text{Li}(N) C_N}{\log N^{1/2-\delta}} \qquad \leq 8\{1 - x_1\}\Theta(N)$$

where x_1 is the first element of the vector $\mathbf{X}$ (3.34).

Thus, Wu obtains an upper bound for Chen's constant.

Chapter 4

Approximating the Buchstab function

In this section we examine how the Buchstab Function $\omega(u)$ (which appears in most of Wu's integrals) is computed.

4.1 Background

The Buchstab function is defined by the following delay differential equation*

$$\begin{aligned} \omega(u) &= 1/u & 1 \le u \le 2, \\ (u\omega(u))' &= \omega(u-1) & u \ge 2. \end{aligned} \tag{4.1}$$

From the graph it appears that $\omega(u)$ quickly approaches a constant value. Buchstab [4] showed that

$$\lim_{u\to\infty} \omega(u) = e^{-\gamma}, \tag{4.2}$$

(where γ is the Euler–Mascheroni constant) and that the convergence is faster than exponential, i.e

$$|\omega(u) - e^{-\gamma}| = O(e^{-u}). \tag{4.3}$$

Hua [24] gave a much stronger bound

$$|\omega(u) - e^{-\gamma}| \le e^{-u(\log u + \log\log u + (\log\log u/\log u) - 1) + O(u/\log u)}. \tag{4.4}$$

*The definition of $\omega(u)$ is very similar to the other difference equations F and f (3.5) and (3.6).

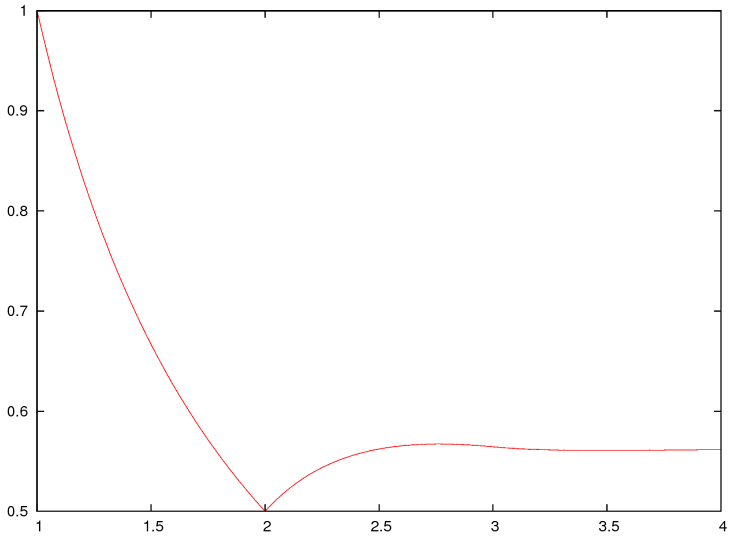


Figure 4.1: Plot of the Buchstab Function $\omega(u)$ for $1 \leq u \leq 4$.

A slightly stronger bound was obtained numerically in *Mathematica* over the interval of interest,

$$\forall u \in [2, 10.5], |\omega(u) - e^{-\gamma}| \leq 0.38e^{-1.275u \log u}.$$

The Buchstab function is related to rough numbers; numbers whose prime factors all exceed some value. If we define

$$\mathbf{\Phi}(x, y) = \#\{n \leq x : p|n \Rightarrow p \geq y\}, \tag{4.5}$$

i.e. the number of positive integers with no prime divisors below y, the following limit holds [9]

$$\lim_{y \to \infty} \mathbf{\Phi}(y^u, y)y^{-u} \log y = \omega(u). \tag{4.6}$$

If we define

$$W(u) = \omega(u) - e^{-\gamma},$$

then $W(u)$ mimics a decaying periodic function. The period of the decay is slowly increasing, and is expected to limit to 1. Also, it has been shown that in every interval $[u, u+1]$ of length 1, $W(u)$ has at least one, but no more than two, zeros. [6] If we let $c_0 = 1$, $c_1 = 2$ and $c_2, c_3, \ldots$ denote the critical points of the Buchstab function, [6] we have that $c_1, c_3, c_5, \ldots$ are local minimums that are strictly increasing, and $c_2, c_4, \ldots$ are local maximums that are strictly decreasing, in the sense that

$$\frac{1}{2} = \omega(c_1) < \omega(c_3) < \omega(c_5) < \ldots \tag{4.7}$$

$$1 = \omega(c_0) > \omega(c_2) > \omega(c_4) > \ldots \tag{4.8}$$

This allows us to obtain the trivial bound

$$1/2 \leq \omega(u) \leq 1. \tag{4.9}$$

Importantly, the Buchstab function decays very quickly to a constant, which makes approximating it easy for the purposes of computing Chen's constant. For $1 \leq u \leq 2$, $\omega(u)$ has a closed form, and since it converges so quickly to $e^{-\gamma}$, we can set $\omega(u)$ to be a constant when u is sufficiently large. Cheer–Goldston published a table of the critical points and zeros of $W(u)$, and by using the critical points

$$W(9.72844) = -9.58 \times 10^{-14}, \qquad W(10.52934) = 3.57 \times 10^{-15}$$

we can conclude using (4.7) that

$$\forall u \geq 10, |W(u)| \leq 10^{-13}. \tag{4.10}$$

For the purposes of numerically integrating $\omega(u)$, we only consider the region $2 \leq u \leq 10$, as beyond that, we can set $\omega(u) = e^{-\gamma}$ for $u \geq 10$ and bound the error by (4.10).

4.2 A piecewise Taylor expansion

A closed form for the Buchstab function can be defined in a piecewise manner for each interval $n \leq u \leq n+1$, as the difference equation can be rearranged such that the value in a particular interval depends on its predecessor.

Theorem 4.2.1. *[6] If we define*

$$\omega_j(u) = \omega(u), \quad j \leq u \leq j+1$$

and integrate (4.1) we obtain

$$u\omega_{j+1}(u) = \int_j^{u-1} \omega_j(t)dt + (j+1)\omega_j(j+1) \quad \text{for } j+1 \leq u \leq j+2. \tag{4.11}$$

Proof. $\omega(u-1)$ is defined for all $u \geq 2$, so by integrating (4.1),

$$u\omega(u) = \int_2^u \omega(t-1)dt,$$

and then by changing variables

$$u\omega(u) = \int_1^{u-1} \omega(t)dt.$$

Restrict u such that $j+1 \le u \le j+2$.

$$\begin{aligned} u\omega_{j+1}(u) &= \int_1^{u-1} \omega_j(t)dt \\ &= \int_j^{u-1} \omega_j(t)dt + \int_1^j \omega(t)dt \\ u\omega_{j+1}(u) - \int_j^{u-1} \omega_j(t)dt &= \int_1^j \omega(t)dt. \end{aligned}$$

Observe that $\int_1^j \omega(t)dt$ is a constant. Call this constant K.

$$\forall u \in [j+1, j+2],\ K = u\omega_{j+1}(u) - \int_j^{u-1} \omega_j(t)dt.$$

Choose $u = j+1$.

$$K = (j+1)\omega_{j+1}(j+1).$$

To force the Buchstab function to be continuous, we assume that the piecewise splines agree at the knots, that is,

$$\omega_j(j+1) = \omega_{j+1}(j+1).$$

So $K = (j+1)\omega_j(j+1)$ and hence

$$u\omega_{j+1}(u) = \int_j^{u-1} \omega_j(t)dt + (j+1)\omega_j(j+1).$$

□

By definition, $\omega_1(u) = u^{-1}$. To obtain $\omega_2(u)$, apply (4.11).

$$\begin{aligned} u\omega_2(u) &= \int_2^{u-1} \omega_1(t)dt + 2\omega_1(2) \\ &= \int_2^{u-1} \frac{1}{t}dt + 2\frac{1}{2} \\ &= \log(u-1) - \log(2-1) + 1 \\ \omega_2(u) &= \frac{\log(u-1)+1}{u}, \quad 2 \le u \le 3. \end{aligned}$$

All values of $\omega_n(u)$ can, in principle, be obtained by repeating the above process, but they cannot be expressed in terms of elementary functions, as

$$\int \frac{\log(u-1)+1}{u} du,$$

is a non-elementary integral. The technique Cheer–Goldston [6] used expresses each $\omega_j(u)$ as a power series about $u = j + 1$.

$$\omega_j(u) = \sum_{k=0}^{\infty} a_k(j)(u - (j+1))^k. \tag{4.12}$$

For the case of $\omega_2(u) = \frac{\log(u-1)+1}{u}$, both $\log(u-1)$ and u^{-1} are analytic, so we may write them in terms of their power series about $u = 3$. Cheer–Goldston shows that by doing this, one obtains

$$a_0(2) = \frac{1 + \log 2}{3}, \tag{4.13}$$

$$a_k(2) = (-1)^{k+1}\left(-\frac{1+\log 2}{3^{k+1}} + \frac{1}{3(2^k)}\sum_{m=0}^{k-1}\frac{1}{k-m}\left(\frac{2}{3}\right)^m\right). \tag{4.14}$$

We note that

$$\sum_{m=0}^{k-1}\frac{1}{k-m}\left(\frac{2}{3}\right)^m \le \sum_{m=0}^{k-1}\left(\frac{2}{3}\right)^m \le \sum_{m=0}^{\infty}\left(\frac{2}{3}\right)^m = 3.$$

Whence it follows that

$$|a_k(2)| \le \left|-\frac{1+\log 2}{3^{k+1}} + \frac{1}{2^k}\right| \le \frac{1}{2^k}.$$

To obtain the value of $a_k(j)$ in general, we follow the method of Marsaglia et al. [35] and substitute (4.12) into (4.11) to obtain

$$u\sum_{k=0}^{\infty} a_k(j+1)(u-(j+2))^k = \int_j^{u-1}\sum_{k=0}^{\infty} a_k(j)(t-(j+1))^k dt + (j+1)a_0(j). \tag{4.15}$$

The Taylor expansion of $\omega_2(u)$ can be shown to converge uniformly in the interval $1.5 \le u \le 4.5$, as

$$|\omega_2(u)| \le \sum_{k=0}^{\infty}|a_k(2)||u-3|^k \le \sum_{k=0}^{\infty}\frac{1}{2^k}|u-3|^k \le \sum_{k=0}^{\infty}\left|\frac{u-3}{2}\right|^k \le \sum_{k=0}^{\infty}\left(\frac{3}{4}\right)^k = 4.$$

Hence by the Weierstrass M-test[15], the series for $\omega_2(u)$ is uniformly convergent for $1.5 \le u \le 4.5$. This allows us to compute the integral of the Taylor series of $\omega_2(u)$, (and thereby compute $\omega_3(u)$) by swapping the order of the sum and the integral, by the Fubini-Tonelli theorem [46]. By using (4.11) we can prove by induction that the Taylor series of $\omega_j(u)$ converges uniformly for $j \le u \le j+1$. This allows interchange of the sums and integrals in (4.15). Thus, we obtain

$$u\sum_{k=0}^{\infty} a_k(j+1)(u-(j+2))^k = (j+1)a_0(j) + \sum_{k=0}^{\infty} a_k(j)\left(\frac{(u-(j+2))^{k+1} - (-1)^{k+1}}{k+1}\right).$$

By making a substitution $x = u - (j+2)$ we obtain

$$\sum_{k=0}^{\infty} a_k(j+1)x^{k+1} + (j+2)\sum_{k=0}^{\infty} a_k(j+1)x^k = (j+1)a_0(j) + \sum_{k=1}^{\infty} \frac{a_{k-1}(j)}{k}\left(x^k + (-1)^{k-1}\right).$$

By subsequently equating coefficients of like terms we obtain the following recursive formula for $a_k(j)$, for all $k \geq 0, j \geq 2$.

$$a_0(j) = a_0(j-1) + \frac{1}{j+1}\sum_{k=1}^{\infty} \frac{(-1)^k}{k+1} a_k(j-1), \tag{4.16}$$

$$a_k(j) = \frac{a_{k-1}(j-1) - k a_{k-1}(j)}{k(j+1)}. \tag{4.17}$$

where the base case $a_k(2)$ and $a_0(2)$ are given in (4.13). Now one can define the Buchstab function in a piecewise manner

$$\omega(u) = \begin{cases} 1/u & 1 \leq u \leq 2, \\ \omega_j(u) & j \leq u \leq j+1. \end{cases} \tag{4.18}$$

4.2.1 Errors of Taylor expansion

In computing $\omega(u)$, we truncate the Taylor expansion to some degree N, and then compute the coefficients of the resulting polynomials to a given accuracy [6]. Denote the approximation of $\omega_2(u)$ as $T_2(u)$, and define the error to be $E_2(u) = \omega_2(u) - T_2(u)$. Define the worst case error as

$$E = \max_{2 \leq u \leq 3} |E_2(u)|.$$

By substuting $T_2(u)$ into (4.11), Cheer [6] shows that one obtains a new approximation $T_3(u)$ for $\omega_3(u)$, with a new error term of

$$\begin{aligned} |E_3(u)| &= \left| \frac{1}{u}\left(\int_2^{u-1} E_2(t)dt + 3E_2(3)\right)\right| \\ &\leq \left| \frac{1}{u}\left(\int_2^{u-1} E dt + 3E\right)\right| = \frac{(u-3)E + 3E}{u} = E. \end{aligned} \tag{4.19}$$

By repeating this argument and then by induction,

$$\forall j \geq 2 \max_{j \leq u \leq j+1} |\omega_j(u) - T_j(u)| = E.$$

So the accuracy of $\omega_2(u)$ holds for the rest of the $\omega_k(u)$, excluding computational errors due to machine precision arithmetic †[6]. (If needed, *Mathematica* supports

†Real number arithmetic on a computer is implemented using floating point numbers, which only have finite accuracy. Hence, every operation introduces rounding errors, and with enough operations, can cause issues with the final result.

arbitrary precision arithmetic, so the magnitude of the computations errors could be made arbitrarily small.)

The error E is easily computed, as by the Taylor remainder theorem [47], for every $u \in [2,3]$ there exists a $\xi \in [2,3]$ such that

$$\omega_2(u) = \sum_{k=0}^{N} a_k(2)(u-3)^k + a_{N+1}(2)(\xi - 3)^{N+1}. \tag{4.20}$$

Then by definition, the error term (for a Taylor expansion to order N) can be written as

$$E_N = \max_{2\leq\xi\leq 3} |a_{N+1}(2)(\xi-3)^{N+1}| \leq |a_{N+1}(2)| \leq \frac{1}{2^{N+1}}. \tag{4.21}$$

So if $\omega_2(u)$ is approximated with a power series up to order N, then the maximum error for $\omega(u)$ anywhere is $2^{-(N+1)}$.

4.2.2 Improving Cheer's Method

The approximation of the Buchstab function was improved, by computing the power series for each $\omega_j(u)$ about $j+0.5$. This way, $\omega_j(u)$ was evaluated at most 0.5 away from the centre of the Taylor expansion. In the previous case, $\omega_j(u)$ could be evaluated up to 1 away from the centre. This provided a much lower error for the same degree Taylor expansion, improving the accuracy of all results using the Buchstab function. By a similar technique as above, by expanding about the middle of each interval $[j, j+1]$ we obtain

$$\omega_j(u) = \sum_{k=0}^{\infty} a_k(j)(u-(j+1/2))^k \quad \text{for } j \leq u \leq j+1, \tag{4.22}$$

where

$$a_k(2) = (-1)^{k+1}\left(-\frac{1+\log\left(\frac{3}{2}\right)}{(5/2)^{k+1}} + \frac{3}{5}\left(\frac{2}{3}\right)^{k+1}\sum_{m=0}^{k-1}\frac{1}{k-m}\left(\frac{3}{5}\right)^m\right), \tag{4.23}$$

$$a_0(j) = \frac{1}{j+1/2}\sum_{k=0}^{\infty}\frac{a_k(j-1)}{2^k}\left(j + \frac{(-1)^k}{2(k+1)}\right), \tag{4.24}$$

$$a_k(j) = \frac{1}{j+1/2}\left(\frac{a_{k-1}(j-1)}{k} - a_{k-1}(j)\right). \tag{4.25}$$

Applying the Taylor remainder theorem, we calculate the error of the Taylor expansion of $\omega_2(u)$, truncated to N terms:

$$E := \max_{2\leq\xi\leq 3} |\omega_2(u) - T_2(u)| \leq |a_{N+1}(2)||(3-2.5)^{N+1}| \leq \frac{1}{2^{N+1}}|a_{N+1}(2)|. \tag{4.26}$$

The coefficient $a_{N+1}(2)$ can be bounded above, as

$$\sum_{m=0}^{k-1} \frac{1}{k-m} \left(\frac{3}{5}\right)^m \leq \sum_{m=0}^{k-1} \left(\frac{3}{5}\right)^m \leq \sum_{m=0}^{\infty} \left(\frac{3}{5}\right)^m = \frac{5}{2}.$$

So,

$$|a_{N+1}(2)| \leq \left| -\frac{1+\log\left(\frac{3}{2}\right)}{(5/2)^{N+2}} + \frac{3}{5}\left(\frac{2}{3}\right)^{N+2} \frac{5}{2} \right| \leq \left(\frac{2}{3}\right)^{N+1}. \tag{4.27}$$

Hence the error bound is improved:

$$E \leq \frac{1}{2^{N+1}} \left(\frac{2}{3}\right)^{N+1} \leq \frac{1}{3^{N+1}}. \tag{4.28}$$

which is better than the old error bound (4.21) by an exponential factor. Again, by a similar argument to (4.19), this error E can be shown to hold everywhere. In practice this is a rather weak error bound, as the actual error is much less. By computing

$$\frac{1}{2^{N+1}} |a_{N+1}(2)|,$$

for $10 \leq N \leq 20$, (rejecting the first few N until the points settle out) and plotting the values on a log plot, we observe the values form a line. By fitting a curve of the form

$$\log y = mx + c,$$

to this line, the asymptotic behaviour of the numerical upper bound error is deduced to be approximately $O(3.31^{-N})$. The base case for the above derivations was done with $\omega_2(u)$ instead of $\omega_1(u)$ as the Taylor expansion of $1/u$ converges slowly. The corresponding error bounds obtained are much weaker. One could, in principle, use $\omega_3(u)$ as the base case and thus obtain a much stronger error bound for $\omega_j(u), j \geq 3$, but as mentioned above, $\omega_3(u)$ is not an elementary function. So, $\omega_2(u)$ is the best we could hope to use. If one used the power series expression of $\omega_3(u)$ to compute the error bounds, each $a_k(3)$ would be defined in terms of

$a_k(2)$ as shown,

$$
\begin{aligned}
a_0(3) &= \frac{1}{3+1/2}\sum_{k=0}^{\infty} a_k(2)2^{-k}\left(j+\frac{(-1)^k}{2(k+1)}\right)\\
&= \frac{1}{3+1/2}\sum_{k=0}^{\infty}\frac{(-1)^{k+1}}{2^k}\left(-\frac{1+\log\left(\frac{3}{2}\right)}{(5/2)^{k+1}}+\frac{3}{5}\left(\frac{2}{3}\right)^{k+1}\sum_{m=0}^{k-1}\frac{1}{k-m}\left(\frac{3}{5}\right)^m\right)\\
&\qquad\left(j+\frac{(-1)^k}{2(k+1)}\right),\\
a_k(3) &= \frac{1}{3+1/2}\left(\frac{a_{k-1}(2)}{k}-a_{k-1}(3)\right).
\end{aligned}
$$

and so, expanded out in full, the formulas for the coefficients would become (even more) unwieldy. Since the error E decreases exponentially quickly with respect to the degree of the polynomial, our implementation of the Buchstab function (given above) was deemed sufficient.

Chapter 5

Numerical computations

We proceeded by implementing the above in *Mathematica*, using the definition of the Buchstab function given in Chapter 4. The approximation to the Buchstab function used is defined as

$$\omega T(u) = \mathbf{1}_{[k+1,\infty)} e^{-\gamma} + \sum_{j=1}^{k} \mathbf{1}_{[j,j+1)} \omega_j(u),$$

where $\omega_j(u)$ is the Taylor polynomial approximation to $\omega(u)$ around $u = j + 1/2$, to some degree N (4.22). The Buchstab function $\omega(u)$ was approximated using a polynomial spline over k intervals, and declared equal to the limit e^{γ} (4.2) beyond the k^{th} interval.

5.1 Justifying Integration Method

We attempted to compute the first of Wu's integrals (3.18) without maximising with respect to ϕ

$$I_1(s, s', \phi) = \iiint\limits_{1/s' \le t \le u \le v \le 1/s} \omega T \left(\frac{\phi - t - u - v}{u} \right) \frac{dt\, du\, dv}{tu^2 v}, \tag{5.1}$$

but ran into several problems. Using *Mathematica*'s inbuilt integration routine, the computation would either finish quickly, or never halt, depending on the value of ϕ chosen. It was discovered that the function could only be integrated for large ϕ, such that $\omega T(u)$ would always be in the constant region. These problems were not resolved. Instead, we integrated the Buchstab function by computing an anti-derivative of $\omega T(u)$, and applying the fundamental theorem of calculus (FTC), three times.

We can show that FTC validly applies in this instance. As $\omega T(u)$ is a piecewise spline of polynomials, it is continuous everywhere except at the points $u = 2, 3, \ldots, k+1$ where the splines meet. Using two theorems about Lebesgue integration [46]

Theorem 5.1.1. *If g is integrable, and $0 \le f \le g$, then f is integrable.*

Theorem 5.1.2. *If f is integrable on $[a, b]$, then there exists an absolutely continuous function F such that $F'(x) = f(x)$ almost everywhere, and in fact we may take $F(x) = \int_a^x f(y)\, dy$.*

The Buchstab function is strictly positive and bounded, as $1/2 \le \omega(u) \le 1$ (4.9). The Taylor approximation $\omega T(u)$ will also be non-negative and bounded, as we can easily bound the difference between $\omega T(u)$ and $\omega(u)$ to be less than any $\epsilon > 0$ (4.28). Thus if $\omega T(u)$ is defined using k many splines, we can bound $\omega T(u)$ above by a constant on the interval $[1, k+1]$. Beyond $u = k+1$, $\omega T(u)$ is constant, so $\omega T(u)$ is integrable on any interval of the form $[1, k+1+r]$ for some $r > 0$. We can thus obtain FTC as

$$F(x) = \int_a^x f(y)\, dy \Rightarrow F(b) - F(a) = \int_a^b f(x)\, dx.$$

We remove the maximisation over ϕ, and set I_1 to be a function dependant on ϕ. We can convert the domain of integration

$$\{(t, u, v) : 1/s' \le t \le u \le v \le 1/s\}$$

into three definite integrals, which is more suitable to apply FTC.

$$\tilde{I}_1(s, s', \phi) = \int_{v=1/s'}^{v=1/s} \int_{t=1/s'}^{t=v} \int_{u=t}^{u=v} \omega T\left(\frac{\phi - t - u - v}{u}\right) \frac{1}{tu^2 v}\, du\, dt\, dv. \tag{5.2}$$

it was expected that the FTC could be used 3 times to compute I_1, however the values computed were nonsense. When attempting to replicate the entry in Wu's table (5.1) for $i = 6$, we expected $0.0094\ldots$ and obtained a large negative result, -10000 or so. It is believed that since $\omega T(u)$ was defined in a piecewise manner, integrating $\omega T\left(\frac{\phi - t - u - v}{u}\right)$ would involve resolving many inequalities, which would only increase in complexity after three integrations.

Attempts to numerically integrate $\omega T(u)$ were successful, however it was much faster to use *Mathematica* to numerically solve the differential delay equation defining the Buchstab function (4.1) with standard numerical ODE solver routines, obtain a numerical solution for $\omega(u)$, and numerically integrate the result.

i	s_i	s'_i	$k_{1,i}$	$k_{2,i}$	$k_{3,i}$	$\Psi_1(s_i)$ (Wu)	$\Psi_1(s_i)$	$\Psi_2(s_i)$ (Wu)	$\Psi_2(s_i)$
1	2.2	4.54	3.53	2.90	2.44			0.01582635	0.01615180
2	2.3	4.50	3.54	2.88	2.43			0.01224797	0.01547663
3	2.4	4.46	3.57	2.87	2.40			0.01389875	0.01406834
4	2.5	4.12	3.56	2.91	2.50			0.01177605	0.01187935
5	2.6	3.58				0.00940521	0.00947409		
6	2.7	3.47				0.00655895	0.00659089		
7	2.8	3.34				0.00353675	0.00354796		
8	2.9	3.19				0.00105665	0.00105838		
9	3.0	3.00				0.00000000	0.00000000		

Table 5.1: Table of values for Ψ_1 and Ψ_2, compared with Wu's results [54].

The resulting values were also closer to Wu's. The following table includes Wu's results, compared to the results we obtained.

Given an s_i, Wu chose the parameters $s'_i, k_{1,i}, k_{2,i}, k_{3,i}$ to maximise $\Psi_1(s_i)$ or $\Psi_2(s_i)$. All the values we calculated were an overshoot of Wu's results, so it was not surprising that we obtained a smaller value for Chen's constant (3.32). For $i = 5, 6, \ldots, 9$, the values of s'_i Wu gave were verified to maximise our version of $\Psi_1(s_i)$, by trying all values $s'_i = 3, 3.01, \ldots, 5.00$, which is given by the constraint $3 \leq s'_i \leq 5$ on (3.17). So even though our Ψ_1 did not match Wu's, both were maximised at the same points. This indicated that we could use our "poor mans" Φ_1 to investigate the behaviour of Φ_1, but not to compute exact values for it.

When computing the values for this table, we first wanted to see for a fixed s and s', how $I_1(s)$ varied as a function of ϕ. It was determined that the function did not grow too quickly near the maximum, and as ϕ grew large, Ψ_1 tended to a constant, which is consistent with $\omega(u)$ quickly tending to $e^{-\gamma}$. Thus, we can apply simple numerical maximisation techniques, without getting trapped in local maxima, or missing the maximum because the function changes too quickly. We only need to maximise ϕ over a small interval $\phi \in [2, 4]$, and we obtain the maximal value by computing I_1 for a few points in the interval of interest, choosing the maximum point, and then computing again for a collection of points in a small neighbourhood about the previous maximum. This is iterated a few times until the required accuracy is obtained. (Listing 5.1).

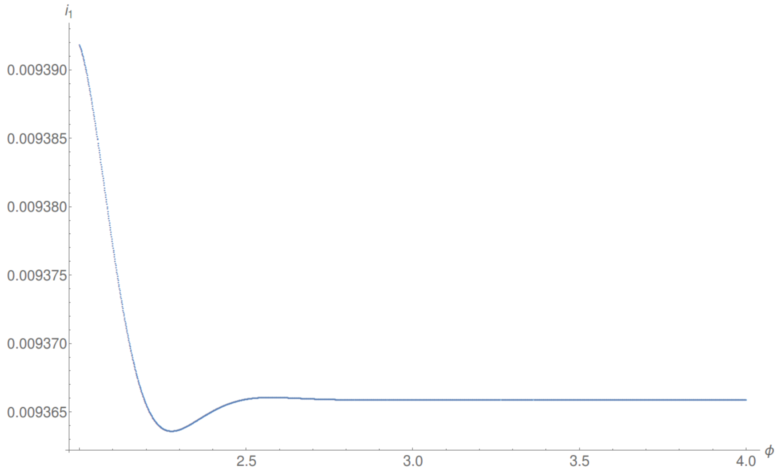


Figure 5.1: Plot of $I_1(\phi, 2.6, 3.58)$ for $2 \leq \phi \leq 4$

```
def I_1(s, s'):
    φ_low := 2
    φ_high := 4
    ε := 0.1
    φ_MAX := 2
    while(ε ≥ 0.001):
        Φ := {φ_low, φ_low + ε, φ_low + 2ε, ..., φ_high}
        φ_MAX := φ ∈ Φ such that Ĩ(φ, s, s') is maximal
            φ_low := max(φ_MAX − ε, 2)
            φ_high := φ_MAX + ε
            ε := ε/10
    return Ĩ_1(φ_MAX, s, s')
enddef
```

Listing 5.1: Algorithm to compute $I_1(s, s')$

Initially, it seemed odd that for all the values of s and s' that were tried, $\tilde{I}_1(\phi, s, s')$ appeared to always be maximal when $\phi = 2$. The actual maximum for $\tilde{I}_1(\phi, s, s')$ occurs at a point $\phi < 2$, but was being cut off by the constraint that $\phi \geq 2$. It seemed unusual to us that Wu would maximise an integral over $\phi \geq 2$, when the integral is always maximal when $\phi = 2$. However, for some of the other integrals in (3.21), the function was maximal at some point $\phi > 2$. This behaviour is made clear when we plot $I_{2,11}(\phi, s = 2.6, s' = 3.58)$ (Figure 5.2) as a function of ϕ, for a fixed value of s and s'.

For some of the integrals needed to compute I_2, the numerical integration

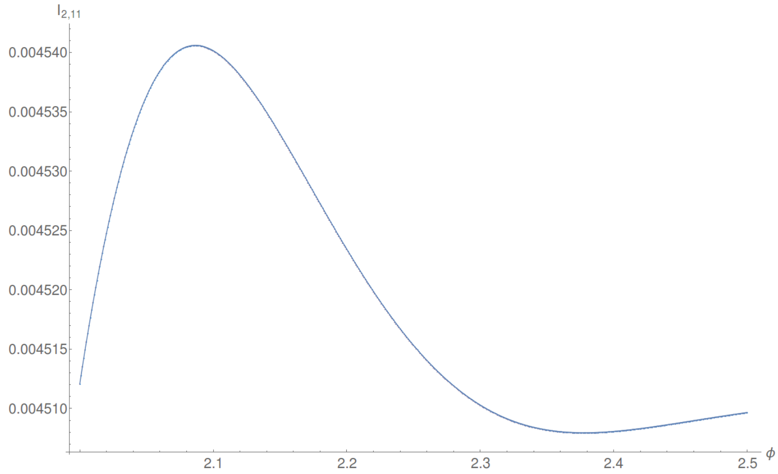


Figure 5.2: Plot of $I_{2,11}$ for $s = 2.6, s' = 3.58, 2 \leq \phi \leq 2.5$

did not converge. Whether this was a property of the integrals (i.e. they were not defined for those particular values of ϕ) or a symptom of how the numerical integration routines in *Mathematica* operate was not determined. To maximise the integrals with respect to ϕ, we could no longer assume they were defined for all $\phi \geq 2$. Instead, it was found that for each integral, there would be a corresponding value ϕ_{low} such that the method of numerical integration converged for all $\phi \geq \phi_{low}$. This value of ϕ_{low} was computed by method of bisection (Listing 5.2).

```
def findphi(i, s, s', k1, k2, k3):
    if(computing I_{2,i}(2, s, s', k1, k2, k3) suceeded):
        return 2
    φ_low := 2
    φ_high := 5
    ε := 0.001
    while(|φ_high − φ_low| ≥ ε):
        φ_mid := (φ_high + φ_low)/2
        if(computing I_{2,i}(φ_mid, s, s', k1, k2, k3) suceeded):
            φ_high := φ_mid
        else:
            φ_low := φ_mid
    return φ_high
enddef
```

Listing 5.2: Algorithm to compute the least ϕ such that $I_{2,i}(\phi, s)$ is defined

I_1 and $I_{2,i}$ can now be computed, and thus Ψ_1 (3.17) and Ψ_2 (3.20) can be easily computed using standard numerical integration techniques. This gives the entries of the vector $\mathbf{B}$ (3.31). Computing the matrix $\mathbf{A}$ (3.31) is comparatively easy, as each element $a_{i,j}$ of the matrix $\mathbf{A}$ is the integral of either Ξ_1 (see 3.16) or Ξ_2 (see 3.16) over an interval, which is easily computed numerically. Thus, the system of linear equations $(\mathbf{I}-\mathbf{A})\mathbf{X}=\mathbf{B}$ (where $\mathbf{I}$ is the identity matrix) can be solved for $\mathbf{X}$. This is compared to the value for $\mathbf{X}$ that Wu obtained.

$$\mathbf{X_{Wu}} = \begin{pmatrix} 0.0223939\ldots \\ 0.0217196\ldots \\ 0.0202876\ldots \\ 0.0181433\ldots \\ 0.0158644\ldots \\ 0.0129923\ldots \\ 0.0100686\ldots \\ 0.0078162\ldots \\ 0.0072943\ldots \end{pmatrix} \qquad \mathbf{X} = \begin{pmatrix} \mathbf{0.022}7656\ldots \\ \mathbf{0.021}9942\ldots \\ \mathbf{0.020}5028\ldots \\ \mathbf{0.018}2930\ldots \\ \mathbf{0.015}2937\ldots \\ \mathbf{0.012}6404\ldots \\ \mathbf{0.0}099076\ldots \\ \mathbf{0.0078}020\ldots \\ \mathbf{0.007}3089\ldots \end{pmatrix} \tag{5.3}$$

So from these vectors, we use (3.34) to obtain two different values for C^*, ours and Wu's,

$$\begin{aligned} C^*_{Wu} &= 8(1-0.0223938) \leq 7.82085, \\ C^* &= 8(1-0.0227655) \leq 7.8178752, \end{aligned} \tag{5.4}$$

which seems to be an improvement on Chen's constant, but since the calculations used to obtain this value are numerical in nature and don't match Wu's results, it can be hard to conclude anything useful from them. Nonetheless, the effect on Chen's constant of sampling s_i with finer granularity was investigated. We could no longer use the table Wu had given (5.1), so we had to numerically optimise over both ϕ and s'_i. Each evaluation of Ψ_2 is very expensive, as we have to compute each of the integrals given in (3.21). This means it is computationally difficult to compute $\Psi_2(s_i)$ without the corresponding parameters $\phi, s'_i, k_{1,i}, k_{2,i}, k_{3,i}$, as for an interval size of n points, we now need to compute n^5 points, which can quickly become infeasible. We focused on increasing the sample size for Ψ_1, by diving the interval of $[2,3]$ into $[2,2.6]\cup[2.6,3.0]$, and increasing the resolution of sampling in the interval $[2.6,3.0]$. By defining

$$s'_i = \begin{cases} 2.1+0.1i & 1 \leq i \leq 4, \\ 2.6+0.01(i-5) & 5 \leq i \leq 45. \end{cases}$$

we use the same values before (See 5.1) for $1 \leq i \leq 4$ and then compute new values of Ψ_1 for each new value of s_i, so we evaluate Ψ_1 at 40 points instead of 5. We can then compute Ψ_1 by numerically maximising over s_i', in a similar fashion to computing I_1 (See Listing 5.1). Note that Ψ_1 depends on I_1, so we are optimising with respect to two variables, ϕ and s_i'. We also need to recompute the matrix $\mathbf{A}$ given by (3.31) on the new set of intervals. Thus, the component $a_{i,j}$ of $\mathbf{A}$ is now given by

$$a_{i,j} := \begin{cases} \displaystyle\int_{s_{j-1}}^{s_j} \Xi_2(t, s_i)dt & i = 1, \ldots, 4;\ j = 1, \ldots, 45 \\ \displaystyle\int_{s_{j-1}}^{s_j} \Xi_1(t, s_i)dt & i = 5, \ldots, 45;\ j = 1, \ldots, 45 \end{cases} \tag{5.5}$$

So we now have a new matrix $\mathbf{A}$ and vector $\mathbf{B}$ with which to solve $(\mathbf{I} - \mathbf{A})\mathbf{X} = \mathbf{B}$.

$$\mathbf{A} := \begin{bmatrix} a_{1,1} & \ldots & a_{1,45} \\ \vdots & \ddots & \vdots \\ a_{45,1} & \ldots & a_{45,45} \end{bmatrix}, \mathbf{B} := \begin{bmatrix} \Psi_2(s_1) \\ \vdots \\ \Psi_2(s_4) \\ \Psi_1(s_5) \\ \vdots \\ \Psi_1(s_{45}) \end{bmatrix} \Rightarrow \mathbf{X} = \begin{pmatrix} 0.0228801\ldots \\ 0.0221067\ldots \\ 0.0206136\ldots \\ 0.0184024\ldots \\ 0.0184024\ldots \\ 0.0153999\ldots \\ 0.0157765\ldots \\ 0.0163132\ldots \\ 0.0170428\ldots \\ \vdots \end{pmatrix}$$

Once that was complete, we redid the calculations again with even finer granularity for s_i', choosing

$$s_i' = \begin{cases} 2.1 + 0.1i & 1 \leq i \leq 5, \\ 2.6 + 0.001(i - 5) & 6 \leq i \leq 405. \end{cases}$$

These calculations were run in parallel on a computer equipped with an i5-3570K CPU overclocked to 3.80Ghz, and with 6GB of RAM. The time taken to compute additional intervals increases rapidly, the projected time for 4000 intervals would take longer than a day to compute, with likely minimal improvement on the constant.

Points	Time **B**	Time **A**	x_1	C^*
Wu	-	-	0.0223938	7.82085
5	1m27s	< 1s	0.0227655	7.8178752
40	11m31s	10s	0.0228800	7.81696
400	1h53m	11m12s	0.0229275	7.81658

Table 5.2: Improvements on C^* by diving $[2.6, 3.0]$ into more points

5.2 Interpolating Wu's data

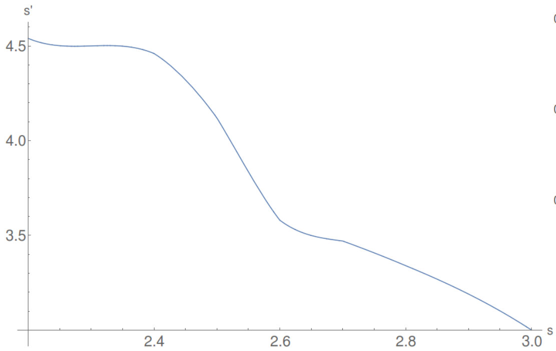
Since Ψ_2 is complicated to evaluate, we looked at approximating it by interpolation, so see what effects additional values of Ψ_2 would have on Chen's constant. We assume the best possible case where possible, to obtain the best possible value for C^*. By demonstrating that even under the best assumptions the improvements on C^* are minimal, this should indicate that improving C^* using Wu's integrals will give a similarly small improvement. Ψ_2 appears to be decreasing by Chen's table, and so too for Ψ_1, so we interpolate the points with *Mathematica* in-built interpolation routine. By plotting the interpolant of Ψ_2 and Ψ_1, we can see one overtakes the other at around $s = 2.55$. This is why Wu had split up his table in this way, choosing Ψ_1 for the lower half and Ψ_2 for the upper, to get the best possible bound.

We define

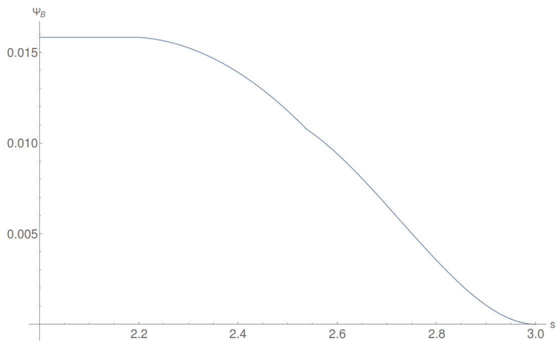
$$\Psi_B = \begin{cases} \Psi_2(s) & s \leq m \\ \Psi_1(s) & s \geq m \end{cases} \tag{5.6}$$

where m is the point where $\Psi_2(m) = \Psi_1(m)$. Thus, Ψ_B is the best case scenario, by essentially taking the maximum of the two upper bounds. We need the values for s', k_1, k_2, k_3 to compute C^*, as we need to compute the matrix $\mathbf{A}$, which in turn depends on the values of $a_{i,j}$ (see 5.5). So we obtain those variables by interpolation also.

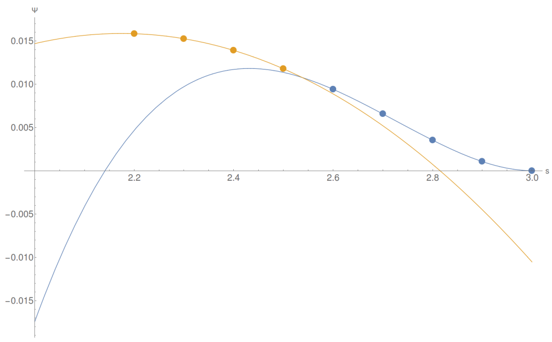
We then discretise the interval $[2, 3]$ from coarse to fine, and calculate the new value of C^* for each of these discretisations. In doing so, we can get an estimate as to how much additional intervals of integration impact the value of C^*. After computing C^* for a varying number of intervals, from Wu's original 9 up to 600 (which took 84 minutes, 40 seconds on the same hardware used to compute Table 5.2), we can clearly see that adding more intervals does make a slight difference, but there are diminishing returns beyond a hundred or so. One would expect not to make any gains on C^* by attempting to compute a million intervals.



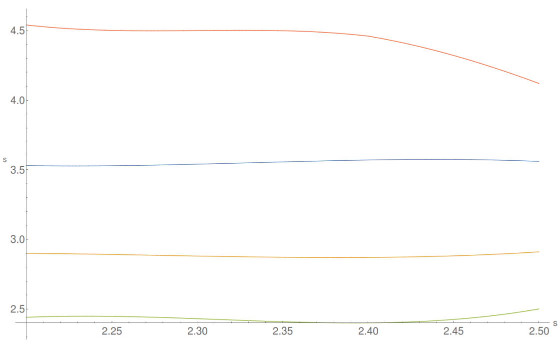
(a) Interpolant for s'



(b) Interpolant of Ψ_B, the best of Ψ_1 and Ψ_2 put together



(c) Interpolant of Ψ_2 (Orange) and Ψ_1 (Blue) from Wu's data



(d) Interpolants for s', k_1, k_2, k_3 (top to bottom)

Figure 5.3: Various interpolants of Wu's data

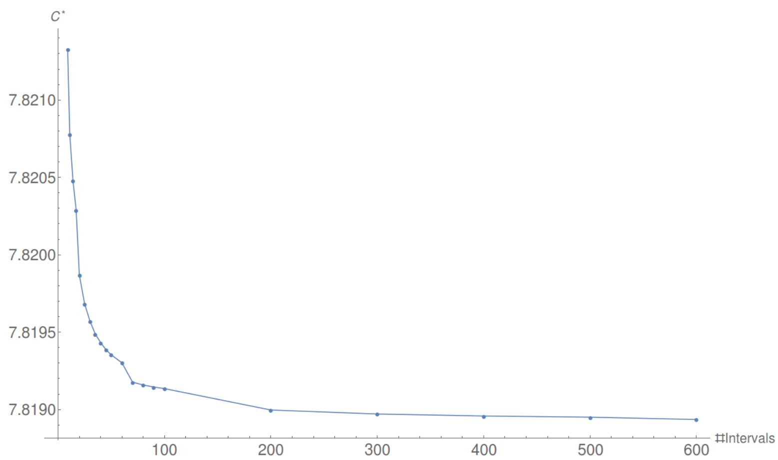


Figure 5.4: Value of C^* versus number of intervals used in integration.

Chapter 6

Summary

6.1 Buchstab function

We have improved on the approximation of the Buchstab function $\omega(u)$ that Cheer–Goldston [6] gave. We used a spline, where each polynomial in the spline is the Taylor expansion of $\omega(u)$ about the centre $u = j + 0.5$ of the interval $[j, j + 1]$, whereas Cheer–Golston expanded about the right endpoint $u = j + 1$ of this interval. We derived an implicit formula for the coefficients $a_j(k)$ for the power series

$$\omega_j(u) = \sum_{k=0}^{\infty} a_j(k)(u - (j + 0.5))^k,$$

where each $a_j(k)$ is defined in terms of the previous values $a_n(m)$ for $2 \leq n < j, 0 \leq m < k$, and the values of $a_2(k)$ are derived from the Taylor expansion of

$$\omega_2(u) = \frac{\log(u - 1) + 1}{u}.$$

The coefficients are more complicated than the ones Cheer–Goldston obtained, but when the Taylor approximation of $\omega(u)$ is truncated to degree N, we show that the corresponding error is less than $1/3^{N+1}$ (4.28) versus Cheer's error bound of $1/2^{N+1}$.

Although the spline is not continuous at the knots, the size of the discontinuities can be made arbitrarily small by increasing the degree of the power series.

6.2 Chen's constant

An attempt was made to use our approximation to the Buchstab function to evaluate the integrals Wu gave, to place an upper bound on C^*. This was not successful, so instead we numerically solved the ODE that defined $\omega(u)$, and numerically evaluated Wu's integrals instead. This gave us approximately the same results as Wu. Wu resolved a set of functional inequalities using a discretisation of $[2, 3]$ into 9 pieces, so we replicated the results, and then increased the resolution for the section $[2.6, 3.0]$ of the interval from 5 points to 40, and then 400. The corresponding change in C^* was as expected, minimal. The relative difference in C^* between sampling 5 points and 400 points in the interval $[2.6, 3.0]$ was only $1.66 \times 10^{-2}\%$. This leads us to believe that we should expect similar results, had we computed an exact form of Wu's integrals.

We interpolated the values of Ψ_1, Ψ_2 and the variables required from Wu's data, and (under the assumption that these interpolations are a reasonable approximation to the exact form), we have shown that Wu was indeed right in asserting that cutting $[2, 3]$ into more subintervals would result in a better value for C^*, but only by a minuscule amount.

Wu gives us that $H(s)$ is decreasing on $[1, 10]$. The constraint on the parameter s is that $2 \leq s \leq 3$, but Wu's discretisation starts at $s = 2.2$. Wu claims this was chosen as Ψ_2 attains its maximum at approximately $s = 2.1$. How close this value of s is to the true maximal value is not stated, so this could be another avenue for improvement. One could explore the value of Ψ_2 in a small neighbourhood around $s = 2.1$, to see what the true maximum is.

Slightly nudging this value left of 2.2 to, say, 2.19 might mean a better upper bound for H, and thus a better value for Chen's constant.

6.3 Future work

There is still a lot of work that could be done to decrease Chen's constant. The obvious improvement is to find a way to compute Ψ^* using the approximation of $\omega(u)$ given above. We could also look at attempting to get the current implementation of Ψ running quicker, which would allow sampling more points in the interval $[2, 2.5]$, and finding the coefficients $\phi, s_i', k_{1,i}, k_{2,i}, k_{3,i}$ that make Ψ_2 maximal, as the current version of Ψ_2 is too slow to optimise over 5 variables simultaneously. We could look at more clever ways to maximise Ψ using more advanced numerical maximisation methods. The behaviour of Ψ is not pathological, in the sense that the functions appear to have some degree of smoothness,

*Whenever Ψ is mentioned in this section, take it to mean both Ψ_1 and Ψ_2.

and the derivative is not too large. It seems true that Ψ are locally concave † near the local maximum, so once values for the variables have been found that bring Ψ near the maximum, one could then run a battery of standard convex optimisation techniques on the problem.

We could also look at alternative forms of approximating $\omega(u)$. Since we are never concerned with the values of $\omega(u)$ at single points, but rather the integral of $\omega(u)$ over intervals, we could look to approximations of $\omega_j(u)$ on each interval $[j, j+1]$ that minimise the L^∞ error

$$||\omega_j(u) - \omega(u)||_{L^\infty[j,j+1]} = \sup_{u \in [j,j+1]} |\omega_j(u) - \omega(u)|,$$

as Taylor expansions are by no means the best polynomial approximation with respect to L^∞ error. Chebyshev ‡ or Hermite § polynomials are ideal for this purpose, and the speed of computing the approximation is not a concern, as we only need to compute the polynomial approximation of $\omega(u)$ once. So the new Chebyshev approximation would be identical to the current approximation, but the polynomials would have different coefficients. We could also look at Bernstein polynomials. ¶

As $\omega(u)$ is continuous, we have by the Weierstrass Approximation Theorem[15] that for any $\epsilon > 0$ and any interval $[1, n]$ there exists a polynomial $p(x)$ such that $||\omega(u) - p(u)||_{L^\infty[1,n]} \leq \epsilon$. Bernstein polynomials provide a constructive way to find such a polynomial $p(x)$. This might prove beneficial as integrating $\omega(\frac{\phi - t - u - v}{u})$ in I_1 (3.18) would prove easier if $\omega(u)$ were represented as a single polynomial instead of a spline, but since $\omega(u)$ is not smooth and in fact has a cusp at $u = 1$, the degree of a polynomial required to closely match $\omega(u)$ to within say 10^6 everywhere could be massive.

†A function f is concave if for any two points $x_1 \leq x_2$, the unique line g that intersects $(x_1, f(x_1))$ and $(x_2, f(x_2))$ satisfies $f(z) \geq g(z)$ for all $x_1 \leq z \leq x_2$.

‡The Chebyshev polynomials are a set of polynomials defined by the recursive formula $T_0(x) = 1, T_1(x) = x, T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x)$. They have the property that the error incurred by using them to approximate a function is more uniformly distributed over the interval the function is being approximated. Taylor series are exact at a single point, and the error tends to grow quickly as points move away from the center of the expansion [5].

§Hermite polynomials are similar to Chebyshev polynomials, but Hermite polynomial approximation also takes into account the derivative of the function being approximated, and attempts to match both the values of the function, and it's derivative [5].

¶The Bernstein polynomials are a family of polynomials, given by $B_n(x) = \sum_{k=0}^{n} \binom{n}{k} x^k (1 - x)^{n-k} f(k/n)$. This is the n^{th} Bernstein polynomial for the function f. It can be shown that $||f - B_n||_{L^\infty([0,1])} \to 0$ i.e. that B_n converges to f uniformly.[15]

None of these piecewise polynomial implementations of $\omega(u)$ would fix the problem of integrating I_1 (3.18), but if that problem were solved, it might permit Wu's values to be more accurately replicated.

For more rigorous ways of showing the difficulty of improving C^*, we could compute some additional points for Wu's table (5.1), and then interpolate the result. The interpolation method did remarkably well at demonstrating the negligible improvements to C^* by a finer discretisation. However, with so few points to interpolate, it is difficult to argue that our interpolant functions for Ψ are actually representative of the behaviour of Ψ. Ideally, we would want to, either by analytic or numeric methods, create an upper bound for Ψ that is in a sense "too good", and then use that to compute C^*. If the resulting value for C^* was only a very small change from Wu's value, then that provides very strong evidence that sizeable improvements on C^* cannot be made by using Wu's method.

Appendix A

All the code used for the results in this thesis was written in *Mathematica*

A.1 Code

Implementation of $D(N)$

```
d[n_] := If[Mod[n/2, 2] == 0, deven[n], dodd[n]]
deven[n_] := Module[{t = 0, p = 2},
     While[p <= n/2, If[PrimeQ[n - p], t++]; p = NextPrime[p]]; t]
dodd[n_] := Module[{t = 0, p = 2},
     While[p <= n/2 - 1, If[PrimeQ[n - p], t++]; p = NextPrime[p]];
  If[PrimeQ[n/2], t++]; t]
```

Taylor expansion of the Buchstab function $\omega(u)$.

```
w2*Exact[u_] := (Log[u - 1] + 1)/u;
degreeT = 10;
precisionT = MachinePrecision;
intervalsT = 5;
wT[1, u_] :=
  Evaluate[N[Normal[Series[1/u, {u, 1 + 1/2, degreeT}]], precisionT]];
wT[2, u_] :=
  Evaluate[N[
    Normal[Series[w2Exact[u], {u, 2 + 1/2, degreeT}]],
    precisionT]];
aw2 =
  N[Evaluate[
    CoefficientList[wT[2, u] /. u -> x + 2 + 1/2, x]],
```

```
   precisionT];
Clear[aw];
aw[k_, 2] := aw2[[k + 1]]
aw[0, j_] :=
 aw[0, j] = (1/(j + 1/2))*
   Sum[(aw[k, j - 1]/2^k)*(j + (-1)^k/(2*(k + 1))),
         {k, 0, degreeT}]
aw[k_, j_] :=
 aw[k, j] = (1/(j + 1/2))*(aw[k - 1, j - 1]/k - aw[k - 1, j])
wT[j_, u_] :=
 ReleaseHold[
  Hold[Sum[aw[k, j]*(u - (j + 1/2))^k, {k, 0, degreeT}]]]
wLim = Exp[-EulerGamma];
wA[u_] := Boole[u > intervalsT + 1]*wLim +
     Sum[Boole[Inequality[k, LessEqual, u, Less, k + 1]]*wT[k,
     u], {k, 1, intervalsT}]
```

Numerical solution to $\omega(u)$.

```
wN[u_] := Evaluate[w[u] /.
NDSolve[{D[u*w[u], u] == w[u - 1], w[u /; u <= 2] == 1/u}, w,
      {u, 1, 30}, WorkingPrecision -> 50]];
```

Defining `unsafeIntegral` to blindly apply FTC without checking for validity.

```
unsafeIntegrate[f_] := f;
unsafeIntegrate[f_, var__,
  rest___] :=
 (unsafeIntegrate[(Integrate[f, var[[1]]] /.
      var[[1]] -> var[[3]]), rest]
   - unsafeIntegrate[(Integrate[f, var[[1]]] /. var[[1]] -> var[[2]]),
     rest])
```

Numerically evaluating I_1 (3.18)

```
i1phiN[p_, sp_, s_] :=
  Quiet[ReleaseHold[NIntegrate[Boole[t <= u <= v]
   *wN[(p - t - u - v)/u]*(1/(t*u^2*v)),
      {u, sp, s}, {t, sp, s}, {v, sp, s}, MaxRecursion -> 10,
```

```
    WorkingPrecision -> MachinePrecision, MaxPoints -> 100000,
     AccuracyGoal -> 20]]][[1]]
```

Numerically evaluating I_{2_i} (3.21)

```
i2[i_, p_, s_, sp_, k1_, k2_, k3_] :=
  Piecewise[{{NIntegrate[Boole[t <= u <= v]
   *wN[(p - t - u - v)/u]*(1/(t*u^2*v)),
       {t, 1/k1, 1/k3}, {u, 1/k1, 1/k3}, {v, 1/k1, 1/k3},
       MaxRecursion -> 10,
       WorkingPrecision -> MachinePrecision, MaxPoints -> 100000,
       AccuracyGoal -> 20][[1]],
     i == 9},
     {NIntegrate[Boole[t <= u]*wN[(p - t - u - v)/u]*(1/(t*u^2*v)),
       {t, 1/k1, 1/k2}, {u, 1/k1, 1/k2}, {v, 1/k2, 1/s},
       MaxRecursion -> 10,
       WorkingPrecision -> MachinePrecision, MaxPoints -> 100000,
       AccuracyGoal -> 20][[1]],
     i == 10},
     {NIntegrate[Boole[u <= v]
      *wN[(p - t - u - v)/u]*(1/(t*u^2*v)),
       {t, 1/k1, 1/k2}, {u, 1/k2, 1/k3}, {v, 1/k2, 1/k3},
       MaxRecursion -> 10,
       WorkingPrecision -> MachinePrecision, MaxPoints -> 100000,
       AccuracyGoal -> 20][[1]],
     i == 11},
     {NIntegrate[Boole[t <= u]*wN[(p - t - u - v)/u]*(1/(t*u^2*v)),
       {t, 1/sp, 1/k1}, {u, 1/sp, 1/k1}, {v, 1/k3, 1/s},
       MaxRecursion -> 10,
       WorkingPrecision -> MachinePrecision, MaxPoints -> 100000,
       AccuracyGoal -> 20][[1]],
     i == 12},
     {NIntegrate[wN[(p - t - u - v)/u]*(1/(t*u^2*v)),
     {t, 1/sp, 1/k1}, {u, 1/k1, 1/k2}, {v, 1/k2, 1/s},
     MaxRecursion -> 10, WorkingPrecision ->
        MachinePrecision, MaxPoints -> 100000,
        AccuracyGoal -> 20][[1]],
        i == 13},
```

```
{NIntegrate[Boole[u <= v]*wN[(p - t - u - v)/u]*(1/(t*u^2*v)),
{t, 1/sp, 1/k1}, {u, 1/k2, 1/s}, {v, 1/k2, 1/s},
MaxRecursion -> 10, WorkingPrecision ->
    MachinePrecision, MaxPoints -> 100000, AccuracyGoal -> 20][[1]],
    i == 14},
{NIntegrate[wN[(p - t - u - v)/u]*(1/(t*u^2*v)),
{t, 1/k1, 1/k2}, {u, 1/k2, 1/k3}, {v, 1/k3, 1/s},
MaxRecursion -> 10, WorkingPrecision -> MachinePrecision,
   MaxPoints -> 100000, AccuracyGoal -> 20][[1]],
   i == 15},
{NIntegrate[Boole[t <= u <= v <= w]
*wN[(p - t - u - v - w)/v]*(1/(t*u*v^2*w)),
   {t, 1/k2, 1/k3}, {u, 1/k2, 1/k3}, {v, 1/k2, 1/k3},
   {w, 1/k2, 1/k3},
   MaxRecursion -> 10, WorkingPrecision -> MachinePrecision,
   MaxPoints -> 100000,
   AccuracyGoal -> 20][[1]],
   i == 16},
{NIntegrate[Boole[t <= u <= v]
*wN[(p - t - u - v - w)/v]*(1/(t*u*v^2*w)),
   {t, 1/k2, 1/k3}, {u, 1/k2, 1/k3}, {v, 1/k2, 1/k3},
   {w, 1/k3, 1/s},
   MaxRecursion -> 10, WorkingPrecision -> MachinePrecision,
   MaxPoints -> 100000,
   AccuracyGoal -> 20][[1]],
   i == 17},
{NIntegrate[Boole[t <= u && v <= w]
*wN[(p - t - u - v - w)/v]*(1/(t*u*v^2*w)),
   {t, 1/k2, 1/k3}, {u, 1/k2, 1/k3},
   {v, 1/k3, 1/s}, {w, 1/k3, 1/s},
   MaxRecursion -> 10, WorkingPrecision -> MachinePrecision,
   MaxPoints -> 100000,
   AccuracyGoal -> 20][[1]], i == 18},
{NIntegrate[Boole[u <= v <= w]
*wN[(p - t - u - v - w)/v]*(1/(t*u*v^2*w)),
   {t, 1/k1, 1/k2}, {u, 1/k3, 1/s}, {v, 1/k3, 1/s},
   {w, 1/k3, 1/s}, MaxRecursion -> 10,
```

```
        WorkingPrecision -> MachinePrecision,
        MaxPoints -> 100000, AccuracyGoal -> 20][[1]],
      i == 19},
      {NIntegrate[Boole[u <= v <= w]
      *wN[(p - t - u - v - w - x)/w]*
         (1/(t*u*v*w^2*x)), {t, 1/k2, 1/k3}, {u, 1/k3, 1/s},
         {v, 1/k3, 1/s}, {w, 1/k3, 1/s},
        {x, 1/k3, 1/s}, MaxRecursion -> 10,
        WorkingPrecision -> MachinePrecision,
        MaxPoints -> 100000,
        AccuracyGoal -> 20][[1]], i == 20},
     {NIntegrate[Boole[t <= u <= v <= w <= x <= y]
      *wN[(p - t - u - v - w - x - y)/x]*
         (1/(t*u*v*w*x^2*y)), {t, 1/k3, 1/s},
         {u, 1/k3, 1/s}, {v, 1/k3, 1/s},
        {w, 1/k3, 1/s}, {x, 1/k3, 1/s}, {y, 1/k3, 1/s},
        MaxRecursion -> 10,
        WorkingPrecision -> MachinePrecision, MaxPoints -> 100000,
        AccuracyGoal -> 20][[1]],
      i == 21}}]
```

Setting up Wu's data

```
k1L[x_] := {3.53, 3.54, 3.57, 3.56}[[x]];
k2L[x_] := {2.9, 2.88, 2.87, 2.91}[[x]];
k3L[x_] := {2.44, 2.43, 2.4, 2.5}[[x]];
sL[i_] := Piecewise[{{1, i == 0}, {2.1 + 0.1*i, i > 0}}];
spL[i_] := {4.54, 4.5, 4.46, 4.12, 3.58, 3.47, 3.34, 3.19, 3.}[[i]];
```

Defining Ψ_2

```
psi2comp[i_, s_, s2_, k1_, k2_,
  k3_] := (-2/5)*Integrate[Log[t - 1]/t, {t, 2, s2 - 1}] -
     (2/5)*Integrate[Log[t - 1]/t, {t, 2, k1 - 1}] -
     (1/5)*Integrate[Log[t - 1]/t, {t, 2, k2 - 1}] +
     (1/5)*
   Integrate[Log[s2*t - 1]/(t*(1 - t)), {t, 1 - 1/s, 1 - 1/s2}] +
```

```
    (1/5)*
   Integrate[Log[k1*t - 1]/(t*(1 - t)), {t, 1 - 1/k3, 1 - 1/k1}] +
    (-2/5)*Sum[i2comp[i, k], {k, 9, 21}]
```

where `i2comp` gives the output of (Listing 5.1)

```
i2comp[i_, k_] := Map[Last, \[Phi]Mout[[i]]][[k - 8]]
```

Part of Ψ_2

```
i2Sum[i_, s_, sp_, k1_, k2_, k3_] :=
   (-2/5)*Sum[i2[k, \[Phi]Max[k, i], sL[i], spL[i],
     k1L[i], k2L[i], k3L[i]], {k, 9, 19}];
```

Implementation of (Listing 5.1), numerical maximisation of I_1 with respect to ϕ.

```
i1testMax[i_, tolmax_] := Module[{tol = 0.1, pMax, pL = pLB[i, k], pH = 5},
   While[tol > tolmax,
     pMax = MaximalBy[monitorParallelTable[Quiet[{p, i2[k, p, sL[i], spL[i], k1L[i],
              k2L[i], k3L[i]]}], {p, pL, pH, tol}, 1], Last][[1]][[1]];
      pL = Max[pMax - tol, 2]; pH = pMax + tol; tol = tol/10];
    {pMax, i2[k, pMax, sL[i], spL[i], k1L[i], k2L[i], k3L[i]]}]
```

Implementation of (Listing 5.2) to find the smallest ϕ such that the integral $I_{2,i}$ is still defined.

```
i1Find[i_, k_, {p_, pL_, pH_, tol_}] :=
  Piecewise[{{2, Quiet[Check[Quiet[i2[k, 2, sL[i], spL[i], k1L[i], k2L[i],
  k3L[i]]],
        "Null"]] != "Null"}, {i2Find2[i, k, {p, pL, pH, tol}], True}}]
i2Find[i_, k_, {p_, pL_, pH_, tol_}] :=
  Piecewise[{{(pH + pL)/2, pH - pL < tol &&
      Quiet[Check[Quiet[i2[k, (pL + pH)/2, sL[i], spL[i], k1L[i], k2L[i], k3L[i]]],
         "Null"]] != "Null"}, {i2Find2[i, k, {p, pL, (pH + pL)/2, tol}],
     Quiet[Check[Quiet[i2[k, (pL + pH)/2, sL[i], spL[i], k1L[i], k2L[i], k3L[i]]],
        "Null"]] != "Null"}, {i2Find2[i, k, {p, (pH + pL)/2, pH, tol}],
     Quiet[Check[i2[k, (pH + pL)/2, sL[i], spL[i], k1L[i], k2L[i], k3L[i]],
     "Null"]] ==
      "Null"}}]
```

```
i2Find[i_, k_, {p_, pL_, pH_, tol_}] :=
  Piecewise[{{2, Quiet[Check[Quiet[i2[k, 2, sL[i], spL[i], k1L[i], k2L[i],
  k3L[i]]],
        "Null"]] != "Null"}, {i2Find2[i, k, {p, pL, pH, tol}], True}}]
i2Find2[i_, k_, {p_, pL_, pH_, tol_}] :=
  Piecewise[{{(pH + pL)/2, pH - pL < tol &&
      Quiet[Check[Quiet[i2[k, (pL + pH)/2, sL[i], spL[i], k1L[i], k2L[i],
      k3L[i]]],
         "Null"]] != "Null"}, {i2Find2[i, k, {p, pL, (pH + pL)/2, tol}],
     Quiet[Check[Quiet[i2[k, (pL + pH)/2, sL[i], spL[i], k1L[i], k2L[i],
     k3L[i]]],
        "Null"]] != "Null"}, {i2Find2[i, k, {p, (pH + pL)/2, pH, tol}],
     Quiet[Check[i2[k, (pH + pL)/2, sL[i], spL[i], k1L[i], k2L[i], k3L[i]],
     "Null"]] ==
      "Null"}}]
```

Computing $a_{i,j}$ (5.5).

```
a1[i_, s_, sp_, k1_, k2_, k3_] := Piecewise[{{k1 - 2, i == 1},
{sp - 2, i == 2},
     {sp - sp/s - 1, i == 3}, {sp - sp/k2 - 1, i == 4},
     {sp - sp/k3 - 1, i == 5},
     {sp - (2*sp)/k2, i == 6}, {sp - sp/k1 - sp/k3, i == 7},
     {sp - sp/k1 - sp/k2, i == 8},
     {k1 - k1/k2 - 1, i == 9}}];
sig0[t_] := sig[3, t + 2, t + 1]/(1 - [3, 5, 4]);
sig[a_, b_, c_] :=
 Evaluate[unsafeIntegrate[(1/t)*Log[c/(t - 1)], {t, a, b}]];
Xi1[t_, s_, sp_] := (0[t]/(2*t))*Log[16/((s - 1)*(sp - 1))] +
    (Boole[sp - 2 <= t <= 3]/(2*t))*Log[(t + 1)^2/((s - 1)*(sp - 1))] +
    (Boole[sp - 2 <= t <= sp - sp/s - 1]/(2*t))*Log[(t + 1)/((s - 1)*
    (sp - 1 - t))];
a1Int[a_, b_, s_, sp_] := NIntegrate[Xi1[t, s, sp], {t, a, b}];
a1[i_, j_] := a1Int[sL[j - 1], sL[j], sL[i], spL[i]];
```

and Ξ_2 (3.23)

```
Xi2[t_, s_, sp_, k1_, k2_, k3_] :=
   (O[t]/(5*t))*Log[1024/((s - 1)*(sp - 1)*(k1 - 1)*(k2 - 1)
   *(k3 - 1))] +
   (Boole[sp - 2 <= t <= 3]/(5*t))*Log[(t + 1)^5/((s - 1)*
   (sp - 1)*(k1 - 1)*(k2 - 1)*(k3 - 1))] +
   (Boole[k1 - k1/k2 - 1 <= t <= k1 - 2]/(5*t))*
     Log[(t + 1)/((k2 - 1)*(k1 - 1 - t))] +
     (Boole[sp - sp/k3 - 1 <= t <= sp - 2]/(5*t))*
     Log[(t + 1)/((k3 - 1)*(sp - 1 - t))] +
     (Boole[sp - sp/s - 1 <= t <= sp - 2]/(5*t))*
     Log[(t + 1)/((s - 1)*(sp - 1 - t))] +
     (Boole[k1 - 2 <= t <= sp - 2]/(5*t))*
     Log[(t + 1)^2/((k1 - 1)*(k2 - 1))] +
     (Boole[sp - sp/k1 - sp/k3 <= t <= sp - sp/k3 - 1]/
      (5*t*(1 - t/sp)))*Log[sp^2/((k1*sp - sp - k1*t)*(k3*sp - sp - k3*t))]
       + (Boole[sp - sp/k3 - 1 <= t <= sp - sp/k1 - sp/k2]/(5*t*(1 - t/sp)))*
     Log[(sp*(sp - 1 - t))/(k1*sp - sp - k1*t)] +
    (Boole[sp - (2*sp)/k2 <= t <= sp - sp/k1 - sp/k2]/(5*t*(1 - t/sp)))*
     Log[sp/(k2*sp - sp - k2*t)] + (Boole[sp - sp/k1 - sp/k2 <= t <= sp - 2]/
      (5*t*(1 - t/sp)))*Log[sp - 1 - t];

a2Int[a_, b_, s_, sp_, k1_, k2_, k3_]
:= NIntegrate[Xi2[t, s, sp, k1, k2, k3], {t, a, b}];

a2[i_, j_] := a2Int[sL[j - 1], sL[j], sL[i], spL[i], k1L[i], k2L[i], k3L[i]];
```

Solving the matrix equations (3.32)

```
bChen = {0.015826357,
  0.015247971,
  0.013898757,
  0.011776059,
  0.009405211,
  0.006558950,
  0.003536751,
  0.001056651,
  0};
```

```
aMat = Table[a[i, j], {i, 1, 9}, {j, 1, 9}];
MatrixForm[LinearSolve[IdentityMatrix[9] - aMat, bVec]]
```

Code to interpolate Wu's data and integrate over d many intervals.

```
psi1data = Table[{sL[i], 1[[i - 4]]}, {i, 5, 9}];
psi2data = Table[{sL[i], 2[[i]]}, {i, 1, 4}];

int1 = Interpolation[psi1data];
int2 = Interpolation[psi2data];

root = s /. FindRoot[int1[s] - int2[s], {s, 2.55}];

interpsi[s_] :=
Piecewise[{{int2[2.2], 2 <= s <= 2.2}, {int2[s], 2.2 <= s <= root},
     {int1[s], root <= s <= 3}}];

spdata = Table[{sL[i], spL[i]}, {i, 1, 9}]
k1data = Table[{sL[i], k1L[i]}, {i, 1, 4}];
k2data = Table[{sL[i], k2L[i]}, {i, 1, 4}];
k3data = Table[{sL[i], k3L[i]}, {i, 1, 4}];

intk1 = Interpolation[k1data];
intk2 = Interpolation[k2data];
intk3 = Interpolation[k3data];
intSp = Interpolation[spdata]

a1Int[a_, b_, s_, sp_] := NIntegrate[Xi1[t, s, sp], {t, a, b}]

sint[i_, d_] := sint[i, d] = Piecewise[{{1, i == 0},
      {Range[22/10, 3, (3 - 22/10)/(d - 1)][[i]], i > 0}}];

a1[i_, j_, d_]
:= a1Int[sint[j - 1, d], sint[j, d], sint[i, d], intSp[sint[i, d]]];

a2Int[a_, b_, s_, sp_, k1_, k2_, k3_]
```

```
:= NIntegrate[Xi2[t, s, sp, k1, k2, k3], {t, a, b}];

a2[i_, j_, d_]
:= a2Int[sint[j - 1, d], sint[j, d], sint[i, d], intSp[sint[i, d]],
    intk1[sint[i, d]], intk2[sint[i, d]], intk3[sint[i, d]]];

a[i_, j_, d_]
:= Piecewise[{{a1[i, j, d], sint[i, d] > root},
     {a2[i, j, d], sint[i, d] < root}}];

aMat[d_] := ParallelTable[a[i, j, d], {i, 1, d}, {j, 1, d}];
bsec[i_, d_] := interpsi[sint[i, d]];
bVec[d_] := Table[interpsi[sint[i, d]], {i, 1, d}];
xVec[d_] := LinearSolve[IdentityMatrix[d] - aMat[d], bVec[d]];
chen[d_] := 8*(1 - xVec[d][[1]])

Quiet[Function[x, AbsoluteTiming[{x, chen[x]}]] /@ {200, 300, 400, 500, 600}]
```

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