

Concrete bounds for Chebyshev's prime counting functions

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Abstract

This entry derives explicit lower and upper bounds for Chebyshev's prime counting functions

$$\psi(x) = \sum_{\substack{p^k \leq x \\ k > 0}} \log p \qquad \vartheta(x) = \sum_{p \leq x} \log p .$$

Concretely, the following inequalities are proven:

- $\psi(x) \geq 0.9x$ for $x \geq 41$
- $\vartheta(x) \geq 0.82x$ if $x \geq 97$
- $\vartheta(x) \leq \psi(x) \leq 1.2x$ if $x \geq 0$

The proofs work by careful estimation of $\psi(x)$, with Stirling's formula as a starting point, to prove the bound for all $x \geq x_0$ with a concrete x_0 , followed by brute-force approximation for all x below x_0 .

An easy corollary of this is *Bertrand's postulate*, i.e. the fact that for any $x > 1$ the interval $(x, 2x)$ contains at least one prime (a fact that has already been shown in the AFP using weaker bounds for ψ and ϑ).

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1 Concrete bounds for Chebyshev's prime counting functions

```
theory Chebyshev_Prime_Exhaust
imports
  "HOL-Decision_Procs.Approximation"
  "HOL-Library.Code_Target_Natural"
  "Prime_Number_Theorem.Prime_Counting_Functions"
begin
```

The well-known Prime Number Theorem states that $\psi(x) \sim \theta(x) \sim x$, i.e. that both $\psi(x)$ and $\vartheta(x)$ are bounded by $(1 \pm \varepsilon)x$ for sufficiently large x for any $\varepsilon > 0$. However, these are asymptotic bounds without giving any concrete information on how ψ and ϑ behave for small x , or even how big x must be until these bound shold.

To complement this, we shall prove some concrete, non-asymptotic bounds. Concretely:

- $\psi(x) \geq 0.9x$ if $x \geq 41$
- $\theta(x) \geq 0.82x$ if $x \geq 97$
- $\theta(x) \leq \psi(x) \leq 1.2x$ if $x \geq 0$

Our formalisation loosely follows a blog entry by A.W. Walker: <https://awwalker.com/2017/02/05/notes-on-the-chebyshev-theorem/>

1.1 Brute-force checking of bounds for ψ and ϑ

1.1.1 Computing powers of a number

```
function powers_below_aux :: "nat  $\Rightarrow$  nat  $\Rightarrow$  nat  $\Rightarrow$  nat list" where
  "powers_below_aux ub n acc = (if acc = 0  $\vee$  n  $\leq$  1  $\vee$  acc > ub then []
else
  acc # powers_below_aux ub n (acc * n))"
  <proof>
termination
  <proof>

lemmas [simp del] = powers_below_aux.simps

lemma set_powers_below_aux:
  assumes "acc > 0" "n > 1"
  shows "set (powers_below_aux ub n acc) = range ( $\lambda i. acc * n ^ i$ )
 $\cap$  {..ub}"
  <proof>

definition powers_below :: "nat  $\Rightarrow$  nat  $\Rightarrow$  nat list" where
```

"powers_below ub n = powers_below_aux ub n n"

lemma set_powers_below:

assumes "n > 1"

shows "set (powers_below ub n) = ($\lambda i. n \wedge i$) ' {1..} \cap {..ub}"

<proof>

lemma distinct_powers_below_aux:

assumes "n > 1" "acc > 0"

shows "distinct (powers_below_aux ub n acc)"

<proof>

lemma distinct_powers_below: "n > 1 \implies distinct (powers_below ub n)"

<proof>

lemma hd_powers_below_aux:

assumes "acc \leq ub" "n > 1" "acc > 0"

shows "hd (powers_below_aux ub n acc) = acc"

<proof>

lemma hd_powers_below:

assumes "n \leq ub" "n > 1"

shows "hd (powers_below ub n) = n"

<proof>

1.1.2 Computing prime powers

definition prime_powers_upto :: "nat \Rightarrow (nat \times nat) list" where

"prime_powers_upto n =

sort_key fst (concat (map ($\lambda p. \text{map } (\lambda k. (k, p))$) (powers_below n p))

(primes_upto n)))"

lemma map_key_sort_key: "map f (sort_key f xs) = sort (map f xs)"

<proof>

lemma distinct_prime_powers_upto:

"distinct (map fst (prime_powers_upto n))"

<proof>

lemma sorted_prime_powers_upto:

"sorted (map fst (prime_powers_upto n))"

<proof>

lemma set_prime_powers_upto:

"set (prime_powers_upto n) = {(q, a) | q. primepow q \wedge q \leq n}"

<proof>

1.1.3 A generic checking function

```

locale chebyshev_check =
  fixes f :: "nat  $\Rightarrow$  real"
    and F :: "nat  $\Rightarrow$  'a  $\Rightarrow$  float"
    and A :: "nat set"
    and plus :: "nat  $\Rightarrow$  float  $\Rightarrow$  float  $\Rightarrow$  float"
    and rel :: "real  $\Rightarrow$  real  $\Rightarrow$  bool"
    and P :: "nat  $\Rightarrow$  real  $\Rightarrow$  bool"
    and num :: "'a  $\Rightarrow$  nat"
  assumes plus: " $\bigwedge$ prec. rel X x  $\Longrightarrow$  rel Y y  $\Longrightarrow$  rel (plus prec X Y)
    (x + y)"
  assumes P_rel: " $\bigwedge$ x y k. P k x  $\Longrightarrow$  rel x y  $\Longrightarrow$  P k y"
  assumes rel_0: "rel 0 0"
  assumes A: "0  $\notin$  A"
begin

definition S where "S n = ( $\sum_{k \in A \cap \{..n\}}$  f k)"
definition S' where "S' n = ( $\sum_{k \in A \cap \{..<n\}}$  f k)"

context
  fixes prec :: nat
begin

function check_aux :: "'a list  $\Rightarrow$  nat  $\Rightarrow$  nat  $\Rightarrow$  float  $\Rightarrow$  nat  $\Rightarrow$  bool"
where
  "check_aux ps lb ub acc n = (if n > ub then True else
    (let (acc', ps') =
      (if ps  $\neq$  []  $\wedge$  num (hd ps) = n then
        (plus prec acc (F prec (hd ps)), tl ps)
      else (acc, ps))
    in (n < lb  $\vee$  P n (real_of_float acc'))  $\wedge$  check_aux ps' lb ub acc'
    (n+1)))"
  <proof>
termination
  <proof>

definition check :: "'a list  $\Rightarrow$  nat  $\Rightarrow$  nat  $\Rightarrow$  bool" where
  "check xs lb ub =
    check_aux xs lb ub 0 (if xs = [] then lb else min lb (num (hd xs)))"

lemmas [simp del] = check_aux.simps

lemma check_aux_correct:
  assumes "sorted (map num ps)" "distinct (map num ps)"
  assumes " $\bigwedge$ p. p  $\leq$  ub  $\Longrightarrow$  p  $\in$  num ' set ps  $\longleftrightarrow$  p  $\in$  A  $\wedge$  p  $\geq$  n"
  assumes " $\bigwedge$ x. x  $\in$  set ps  $\Longrightarrow$  rel (real_of_float (F prec x)) (f (num
x))"
  assumes "rel (real_of_float acc) (S' n)"
  assumes "check_aux ps lb ub acc n"

```

```

    assumes "k ∈ {max lb n..ub}"
    shows   "P k (S k)"
    ⟨proof⟩

lemma check_correct:
  assumes "sorted (map num ps)" "distinct (map num ps)"
  assumes "∧p. p ≤ ub ⇒ p ∈ num ' set ps ↔ p ∈ A"
  assumes "∧x. x ∈ set ps ⇒ rel (real_of_float (F prec x)) (f (num
x))"
  assumes "check ps lb ub"
  assumes "k ∈ {lb..ub}"
  shows   "P k (S k)"
  ⟨proof⟩

end

end

```

1.1.4 The ϑ function

context

begin

interpretation primes_theta: chebyshev_check

```

  "λn. ln (real n)"
  "λprec n. the (lb_ln prec (Float (int n) 0))"
  "{p. prime p}"
  "float_plus_down"
  "(≤)"
  "λk x. x ≥ c * (real k + 1)"
  "λn. n"
  for c :: real
  ⟨proof⟩

```

definition check_theta_lower_aux

```

  where "check_theta_lower_aux = primes_theta.check_aux"

```

definition check_theta_lower where

```

  "check_theta_lower c prec lb ub =
    primes_theta.check c prec (primes_upto ub) lb ub"

```

lemma check_theta_lower_aux_code [code]:

```

  "check_theta_lower_aux c prec ps lb ub acc n =
    (if ub < n then True else let (acc', ps') =
      if ps ≠ [] ∧ hd ps = n
      then (float_plus_down prec acc (the (lb_ln prec (Float (int
(hd ps)) 0))), tl ps)
      else (acc, ps)

```

```

    in (n < lb  $\vee$  c * (real n + 1)  $\leq$  real_of_float acc')  $\wedge$ 
      check_theta_lower_aux c prec ps' lb
      ub acc' (n + 1))"
  <proof>

lemma check_theta_lower_code [code]:
  "check_theta_lower c prec lb ub = (let ps = primes_upto ub in
    check_theta_lower_aux c prec ps lb ub 0
    (if ps = [] then lb else min lb (hd ps)))"
  <proof>

lemma check_theta_lower_correct:
  assumes "check_theta_lower c prec lb ub"
  shows " $\forall x \in \{\text{real lb}.. \text{real ub}\}. \text{primes\_theta } x \geq c * x$ "
  <proof>

end

context
begin

interpretation primes_theta: chebyshev_check
  " $\lambda n. \ln (\text{real } n)$ "
  " $\lambda \text{prec } n. \text{the } (\text{ub\_ln } \text{prec } (\text{Float } (\text{int } n) 0))$ "
  "{p. prime p}"
  "float_plus_up"
  " $(\geq)$ "
  " $\lambda k x. x \leq c * \text{real } k$ "
  " $\lambda n. n$ "
  for c :: real
  <proof>

definition check_theta_upper_aux
  where "check_theta_upper_aux = primes_theta.check_aux"

definition check_theta_upper where
  "check_theta_upper c prec lb ub =
    primes_theta.check c prec (primes_upto ub) lb ub"

lemma check_theta_upper_aux_code [code]:
  "check_theta_upper_aux c prec ps lb ub acc n =
    (if ub < n then True else let (acc', ps') =
      if ps  $\neq$  []  $\wedge$  hd ps = n
      then (float_plus_up prec acc (the (ub_ln prec (Float (int
        (hd ps)) 0))), tl ps)

```

```

      else (acc, ps)
    in (n < lb  $\vee$  c * real n  $\geq$  real_of_float acc')  $\wedge$ 
      check_theta_upper_aux c prec ps' lb
      ub acc' (n + 1))"
  <proof>

lemma check_theta_upper_code [code]:
  "check_theta_upper c prec lb ub = (let ps = primes_upto ub in
    check_theta_upper_aux c prec ps lb ub 0
    (if ps = [] then lb else min lb (hd ps)))"
  <proof>

lemma check_theta_upper_correct:
  assumes "check_theta_upper c prec lb ub" "c  $\geq$  0"
  shows " $\forall x \in \{\text{real lb}.. \text{real ub}\}. \text{primes\_theta } x \leq c * x$ "
  <proof>

end

1.1.5 The  $\psi$  function

context
begin

interpretation primes_psi: chebyshev_check
  " $\lambda n. \ln (\text{real } (\text{aprime divisor } n))$ "
  " $\lambda \text{prec } x. \text{the } (\text{lb\_ln } \text{prec } (\text{Float } (\text{int } (\text{snd } x)) 0))$ "
  "{p. primepow p}"
  "float_plus_down"
  " $(\leq)$ "
  " $\lambda k x. x \geq c * (\text{real } k + 1)$ "
  "fst"
  for c :: real
  <proof>

definition check_psi_lower_aux
  where "check_psi_lower_aux = primes_psi.check_aux"

definition check_psi_lower where
  "check_psi_lower c prec lb ub =
    primes_psi.check c prec (prime_powers_upto ub) lb ub"

lemma check_psi_lower_aux_code [code]:
  "check_psi_lower_aux c prec ps lb ub acc n =
    (if ub < n then True else let (acc', ps') =
      if ps  $\neq$  []  $\wedge$  fst (hd ps) = n
      then (float_plus_down prec acc (the (lb_ln prec (Float (int
        (snd (hd ps)))) 0))), tl ps)
```

```

      else (acc, ps)
    in (n < lb  $\vee$  c * (real n + 1)  $\leq$  real_of_float acc')  $\wedge$ 
      check_psi_lower_aux c prec ps' lb
      ub acc' (n + 1))"
  <proof>

lemma check_psi_lower_code [code]:
  "check_psi_lower c prec lb ub = (let ps = prime_powers_upto ub in
    check_psi_lower_aux c prec ps lb ub 0
    (if ps = [] then lb else min lb (fst (hd ps))))"
  <proof>

lemma check_psi_lower_correct:
  assumes "check_psi_lower c prec lb ub"
  shows " $\forall x \in \{\text{real lb}.. \text{real ub}\}. \text{primes\_psi } x \geq c * x$ "
  <proof>

end

context
begin

interpretation primes_psi: chebyshev_check
  " $\lambda n. \ln (\text{real } (\text{aprime divisor } n))$ "
  " $\lambda \text{prec } x. \text{the } (\text{ub\_ln prec } (\text{Float } (\text{int } (\text{snd } x)) 0))$ "
  "{p. primepow p}"
  "float_plus_up"
  " $(\geq)$ "
  " $\lambda k x. x \leq c * \text{real } k$ "
  "fst"
  for c :: real
  <proof>

definition check_psi_upper_aux
  where "check_psi_upper_aux = primes_psi.check_aux"

definition check_psi_upper where
  "check_psi_upper c prec lb ub =
    primes_psi.check c prec (prime_powers_upto ub) lb ub"

lemma check_psi_upper_aux_code [code]:
  "check_psi_upper_aux c prec ps lb ub acc n =
    (if ub < n then True else let (acc', ps') =
      if ps  $\neq$  []  $\wedge$  fst (hd ps) = n
      then (float_plus_up prec acc (the (ub_ln prec (Float (int
(snd (hd ps))) 0))), tl ps)
      else (acc, ps)

```



```

    in (n < lb  $\vee$  c * real n  $\geq$  real_of_float acc')  $\wedge$ 
      check_psi_upper_aux c prec ps' lb
      ub acc' (n + 1))"
  <proof>

lemma check_psi_upper_code [code]:
  "check_psi_upper c prec lb ub = (let ps = prime_powers_upto ub in
    check_psi_upper_aux c prec ps lb ub 0
    (if ps = [] then lb else min lb (fst (hd ps))))"
  <proof>

lemma check_psi_upper_correct:
  assumes "check_psi_upper c prec lb ub" "c  $\geq$  0"
  shows " $\forall x \in \{\text{real lb}.. \text{real ub}\}. \text{primes\_psi } x \leq c * x$ "
  <proof>

end

end
theory Chebyshev_Prime_Bounds
imports
  "Prime_Number_Theorem.Prime_Counting_Functions"
  "Prime_Distribution_Elementary.Prime_Distribution_Elementary_Library"
  "Prime_Distribution_Elementary.Primorial"
  "HOL-Decision_Procs.Approximation"
  "HOL-Library.Code_Target_Natural"
  Chebyshev_Prime_Exhaust
begin



## 1.2 Auxiliary material



context comm_monoid_set
begin

lemma union_disjoint':
  assumes "finite C" "A  $\cup$  B = C" "A  $\cap$  B = {}"
  shows "f (F g A) (F g B) = F g C"
  <proof>

end

lemma sum_mset_nonneg:
  fixes X :: "'a :: ordered_comm_monoid_add multiset"
  shows " $(\bigwedge x. x \in \# X \implies x \geq 0) \implies \text{sum\_mset } X \geq 0$ "
  <proof>

lemma of_int_sum_mset: "of_int (sum_mset M) = sum_mset (image_mset of_int
M)"
  <proof>

```

```
lemma sum_sum_mset: "( $\sum_{x \in A}. \sum_{y \in \#B}. f\ x\ y$ ) = ( $\sum_{y \in \#B}. \sum_{x \in A}. f\ x\ y$ )"
  <proof>
```

```
lemma sum_mset_diff_distrib:
  fixes f g :: "'a  $\Rightarrow$  'b :: ab_group_add"
  shows "( $\sum_{x \in \#A}. f\ x - g\ x$ ) = ( $\sum_{x \in \#A}. f\ x$ ) - ( $\sum_{x \in \#A}. g\ x$ )"
  <proof>
```

```
lemma sum_mset_neg_distrib:
  fixes f :: "'a  $\Rightarrow$  'b :: ab_group_add"
  shows "( $\sum_{x \in \#A}. -f\ x$ ) = -( $\sum_{x \in \#A}. f\ x$ )"
  <proof>
```

1.3 Bounds for the remainder in Stirling's approximation

```
definition ln_fact_remainder :: "real  $\Rightarrow$  real" where
  "ln_fact_remainder x = ln (fact (nat  $\lfloor$ x $\rfloor$ )) - (x * ln x - x)"
```

```
lemma ln_fact_remainder_bounds:
  assumes x: "x  $\geq$  3"
  shows "ln_fact_remainder x  $\leq$  ln x / 2 + ln (2 * pi) / 2 + 1 / (12 *  $\lfloor$ x $\rfloor$ )"
  and "ln_fact_remainder x  $\geq$  -ln x / 2 + ln (2 * pi) / 2 - 1 / (2 * x)"
  <proof>
```

```
lemma abs_ln_fact_remainder_bounds:
  assumes x: "x  $\geq$  3"
  shows "|ln_fact_remainder x| < ln x / 2 + 1"
  <proof>
```

1.4 Approximating ψ

```
unbundle prime_counting_notation
```

```
lemma primes_psi_lower_rec:
  fixes f :: "real  $\Rightarrow$  real"
  assumes " $\bigwedge x. x \geq x_0 \implies f\ x \leq f\ (x / c) + h\ x$ "
  assumes "x0 > 0" "x * c  $\geq$  x0 * c ^ n" "c  $\geq$  1"
  shows "f x  $\leq$  f (x / c ^ n) + ( $\sum_{k < n}. h\ (x / c ^ k)$ )"
  <proof>
```

```
locale chebyshev_multiset =
  fixes L :: "int multiset"
  assumes L_nonzero: "0  $\notin$  # L"
begin
```

```

definition chi_L :: "real  $\Rightarrow$  int" (" $\chi_L$ ")
  where "chi_L t = ( $\sum_{l \in \#L}. \text{sgn } l * \lfloor t / |l| \rfloor$ )"

definition psi_L :: "real  $\Rightarrow$  real" (" $\psi_L$ ")
  where "psi_L x = sum_upto ( $\lambda d. \text{mangoldt } d * \text{chi}_L (x / d)$ ) x"

definition alpha_L :: real (" $\alpha_L$ ")
  where "alpha_L = -( $\sum_{l \in \#L}. \ln |l| / l$ )"

definition period :: nat
  where "period = nat (Lcm (set_mset L))"

lemma period_pos: "period > 0"
  <proof>

lemma dvd_period: "l  $\in \# L \implies l$  dvd period"
  <proof>

lemma chi_L_decompose:
  " $\chi_L (x + \text{of\_int } (m * \text{int period})) = \chi_L x + m * \text{int period} * (\sum_{l \in \#L}. 1 / l)$ "
  <proof>

lemma chi_L_floor: "chi_L (floor x) = chi_L x"
  <proof>

end

locale balanced_chebyshev_multiset = chebyshev_multiset +
  assumes balanced: " $(\sum_{l \in \#L}. 1 / l) = 0$ "
begin

lemma chi_L_mod: " $\chi_L (\text{of\_int } (a \bmod \text{int period})) = \chi_L (\text{of\_int } a)$ "
  <proof>

sublocale chi: periodic_fun_simple chi_L "of_int period"
  <proof>

definition psi_L_remainder where
  " $\text{psi}_L\text{-remainder } x = (\sum_{l \in \#L}. \text{sgn } l * \text{ln\_fact\_remainder } (x / |l|))$ "

lemma abs_sum_mset_le:
  fixes f :: "'a  $\Rightarrow$  'b :: ordered_ab_group_add_abs"
  shows " $|\sum_{x \in \#A}. f x| \leq (\sum_{x \in \#A}. |f x|)$ "
  <proof>

lemma psi_L_remainder_bounds:

```

```

fixes x :: real
assumes x: "x ≥ 3" "∧l. l ∈# L ⇒ x ≥ 3 * |l|"
shows "|psi_L_remainder x| ≤
      ln x * size L / 2 - 1/2 * (∑ l∈#L. ln |l|) + size L"
⟨proof⟩

lemma psi_L_eq:
  assumes "x > 0"
  shows "psi_L x = α_L * x + psi_L_remainder x"
⟨proof⟩

lemma primes_psi_lower_bound:
  fixes x C :: real
  defines "x0 ≡ Max (insert 3 ((λl. 3 * |l|) ` set_mset L))"
  assumes x: "x ≥ x0"
  assumes chi_le1: "∧n. n ∈ {0..<period} ⇒ χ_L (real n) ≤ 1"
  defines "C ≡ 1 / 2 * (∑ l∈#L. ln |l|) - size L"
  shows "ψ x ≥ α_L * x - ln x * size L / 2 + C"
⟨proof⟩

end

lemma psi_lower_bound_precise:
  assumes x: "x ≥ 90"
  shows "ψ x ≥ 0.92128 * x - 2.5 * ln x - 1.6"
⟨proof⟩

context balanced_chebyshev_multiset
begin

lemma psi_upper_bound:
  fixes x c C :: real
  defines "x0 ≡ Max ({3, 55 * c} ∪ {3 * |l| | l. l ∈# L})"
  assumes x: "x ≥ x0"
  assumes chi_nonneg: "∧n. n ∈ {0..<period} ⇒ χ_L (real n) ≥ 0"
  assumes chi_ge1: "∧n. real n ∈ {1..<c} ⇒ χ_L (real n) ≥ 1"
  assumes c: "c > 1" "c ≤ period"
  assumes "α_L ≥ 0"
  shows "ψ x ≤ c / (c - 1) * α_L * x + (3 * size L) / (4 * ln c) * ln
x ^ 2 + ψ x0"
⟨proof⟩

end

```

1.5 Final results

```

theorem psi_lower_ge_9:
  assumes x: "x ≥ 41"
  shows "ψ x ≥ 0.9 * x"

```

<proof>

theorem *primes_theta_ge_82:*

assumes " $x \geq 97$ "

shows " $\exists x \geq 0.82 * x$ "

<proof>

corollary *primorial_ge_exp_82:*

assumes " $x \geq 97$ "

shows " $\text{primorial } x \geq \exp (0.82 * x)$ "

<proof>

theorem *primes_psi_le_111:*

assumes " $x \geq 0$ "

shows " $\psi x \leq 1.11 * x$ "

<proof>

corollary *primes_theta_le_111:*

assumes " $x \geq 0$ "

shows " $\exists x \leq 1.11 * x$ "

<proof>

As an easy corollary, we obtain Bertrand's postulate: For any real number $x > 1$, the interval $(x, 2x)$ contains at least one prime.

corollary *bertrands_postulate:*

assumes " $x > 1$ "

shows " $\exists p. \text{prime } p \wedge \text{real } p \in \{x < .. < 2 * x\}$ "

<proof>

unbundle *no_prime_counting_notation*

end