



Article Considering a Classical Upper Bound on the Frobenius Number

Aled Williams *,[†] and Daiki Haijima [†]

Department of Mathematics, London School of Economics and Political Science, London WC2B 4RR, UK * Correspondence: a.e.williams1@lse.ac.uk

⁺ These authors contributed equally to this work.

Abstract: In this paper, we study the (classical) Frobenius problem, namely the problem of finding the largest integer that cannot be represented as a nonnegative integer combination of given, relatively prime, (strictly) positive integers (known as the Frobenius number). The main contribution of this paper are observations regarding a previously known upper bound on the Frobenius number where, in particular, we observe that a previously presented argument features a subtle error, which alters the value of the upper bound. Despite this, we demonstrate that the subtle error does not impact upon on the validity of the upper bound, although it does impact on the upper bounds tightness. Notably, we formally state the corrected result and additionally compare the relative tightness of the corrected upper bound with the original. In particular, we show that the updated bound is tighter in all but only a relatively "small" number of cases using both formal techniques and via Monte Carlo simulation techniques.

Keywords: Frobenius problem; Frobenius number; Diophantine equations; knapsack problems; knapsack polytopes; integer programming

MSC: 11D07; 11D45; 90C10; 11D75

1. Introduction

Let *a* be a positive integer *n*-dimensional primitive vector, i.e., $\mathbf{a} = (a_1, \ldots, a_n)^T \in \mathbb{Z}_{>0}^n$ with $gcd(\mathbf{a}) := gcd(a_1, \ldots, a_n) = 1$, where $\mathbb{Z}_{>0}^n$ denotes the set of *n*-dimensional vectors with strictly positive integer entries. In what follows, we exclude the case n = 1 and assume that the dimension $n \ge 2$. In particular, without the loss of generality, we assume the following conditions:

$$a = (a_1, \dots, a_n)^T \in \mathbb{Z}_{>0}^n$$
, $n \ge 2$ and $gcd(a) := gcd(a_1, \dots, a_n) = 1.$ (1)

The *Frobenius number* of a, denoted by F(a), is the largest integer that cannot be represented as a nonnegative integer combination of the a_i s, i.e.,

$$F(a) := \max \Big\{ b \in \mathbb{Z} : b \neq a^T z \text{ for all } z \in \mathbb{Z}_{\geq 0}^n \Big\}.$$

where a^T denotes the transpose of a. It should be noted for completeness that the Frobenius problem, namely the problem of finding the Frobenius number, is also known by other names within the literature including the money-changing problem (or the money-changing problem of Frobenius, or the coin-exchange problem of Frobenius) [1–3], the coin problem (or the Frobenius coin problem) [4,5], and the Diophantine problem of Frobenius [6,7]. From a geometric viewpoint, F(a) is the maximal right-hand side $b \in \mathbb{Z}$ such that the *knapsack polytope*

$$P(\boldsymbol{a},\boldsymbol{b}) = \left\{ \boldsymbol{x} \in \mathbb{R}^n_{\geq 0} : \boldsymbol{a}^T \boldsymbol{x} = \boldsymbol{b} \right\}$$



Citation: Williams, A.; Haijima, D. Considering a Classical Upper Bound on the Frobenius Number. *Mathematics* **2024**, *12*, 4029. https:// doi.org/10.3390/math12244029

Academic Editor: Jiyou Li

Received: 17 October 2024 Revised: 10 December 2024 Accepted: 16 December 2024 Published: 22 December 2024



Copyright: © 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (https:// creativecommons.org/licenses/by/ 4.0/). does not contain integer points. Note that P(a, b) is simply the intersection of a hyperplane defined by a and b with the nonnegative orthant. It should be noted that the conditions in (1) are indeed necessary and sufficient conditions for the existence of the Frobenius number.

Note that instead of the conditions in (1), some authors instead assume the stronger condition that all the entries of the vector are pairwise coprime, i.e.,

$$a = (a_1, \dots, a_n)^T \in \mathbb{Z}_{>0}^n$$
, $n \ge 2$ and $gcd(a_i, a_j) = 1$ for any $i, j \in \{1, 2, \dots, n\}$ with $i \ne j$. (2)

It should be noted that not all integer vectors satisfying (1) also satisfy the stronger conditions (2). The vector $\mathbf{a} = (6, 10, 15)^T$, for example, satisfies gcd(6, 10, 15) = 1 but not the pairwise coprime condition, since $gcd(6, 10) \neq 1$.

There is a very rich history on Frobenius numbers and the book [8] provides a very good survey of the problem. It is worth noting that computing the Frobenius number in general is \mathcal{NP} -hard [9] (which was proved via a reduction to the integer knapsack problem); however, if the number of integers *n* is fixed, then a polynomial time algorithm to calculate *F*(*a*) exists [10]. If *n* = 2, it is well known (most likely due to Sylvester [11]) that

$$F(a_1, a_2) = a_1 a_2 - a_1 - a_2$$

= $(a_1 - 1)(a_2 - 1) - 1.$ (3)

In contrast to the case when n = 2, it was shown by Curtis [12] that no closed formula exists for the Frobenius number if n > 2. In light of this, there has been a great deal of research into producing upper bounds on F(a). These bounds share the property that in the worst case they are of a quadratic order with respect to the maximum absolute valued entry of a, which will be denoted by $||a||_{\infty}$. Further, let $|| \cdot ||_2$ denote the Euclidean norm. In particular, upon assuming that $a_1 \le a_2 \le \cdots \le a_n$ holds, such bounds include the classical bound by Erdős and Graham [13] [Theorem 1],

$$F(a) \leq 2a_{n-1} \left\lfloor \frac{a_n}{n} \right\rfloor - a_n,$$

by Selmer [6],

$$F(a) \leq 2a_n \left\lfloor \frac{a_1}{n} \right\rfloor - a_1,$$

by Vitek [14] [Theorem 5],

$$F(a) \leq \frac{1}{2}(a_2-1)(a_n-2)-1,$$

by Beck et al. [15] [Theorem 9],

$$F(a) \leq \frac{1}{2} \left(\sqrt{a_1 a_2 a_3 (a_1 + a_2 + a_3)} - a_1 - a_2 - a_3 \right),$$

and by Fukshansky and Robins [16] [Equation (29)],

$$F(a) \leq \left\lfloor \frac{(n-1)^2 \Gamma(\frac{n+1}{2})}{\pi^{(n-1)/2}} \sum_{i=1}^n a_i \sqrt{\|a\|_2^2 - a_i^2} + 1 \right\rfloor,$$

where $\Gamma(\cdot)$ and $\lfloor \cdot \rfloor$ denote Euler's gamma and the standard floor functions, respectively.

It is worth noting that providing accurate upper bounds in the general setting, namely without additional assumptions on the vector a, is not the only direction of research. In particular, there have been results on lower bounds for F(a) (e.g., [17–19]), some explicit formulas provided in special cases (e.g., [6,20–27]) and algorithms for computing the Frobenius number (e.g., [1,10,28–33]).

Building on these directions of research, this paper is motivated by the need for accurate and reliable upper bounds on the Frobenius number, particularly in settings

with minimal assumptions on the input vector *a*. Such bounds play a crucial role in understanding the complexity of the Frobenius problem and its connections to optimisation problems such as the knapsack (see, e.g., [34] [Chapter 16]) and subset–sum (see, e.g., [34] [Chapter 35]) problems.

This paper focuses on refining a well-known upper bound, originally proposed by Beck et al. [15] [Theorem 9]. While this bound has been cited in the literature, we identify a subtle error in its derivation that, while not invalidating the bound itself, affects its tightness. Our primary contribution is the formal correction of this result, alongside a rigorous comparison of the relative tightness of the corrected and original bounds. Through theoretical analysis and Monte Carlo simulations, we demonstrate that the corrected bound is tighter in "nearly all" cases. This work not only addresses a key issue in the existing literature but also enhances our understanding of the structure of upper bounds under general settings, paving the way for further advancements in this area of research.

2. Preliminary and Auxiliary Results

In this section, we present some preliminary results that are essential for establishing a requirement for upper bounds on F(a) when the more general conditions (1) on a hold. In particular, this requirement is induced via a simple lower bound which considers the parity of the a_i s and is formally introduced below.

Proposition 1. If an integer vector **a** satisfies (1), then at least one a_i must be odd for $i \in \{1, 2, ..., n\}$.

Proof. Suppose for contradiction that there does not exist an odd a_i , i.e., that a has only even elements. It follows immediately that $gcd(a) \ge 2$, which contradicts the assumed conditions in (1), as required. \Box

Denote by $o_t := o_t(a)$ the *t*-th smallest odd element in *a*. Observe that Proposition 1 implies that o_1 necessarily exists for any integer vector *a* satisfying (1).

Proposition 2. If an integer vector a satisfies (1), then $o_1 - 2$ is a lower bound for F(a).

Proof. Firstly, observe that since o_1 is the smallest odd element in a, it follows that any odd number strictly less than o_1 cannot be expressed as $\sum_{i=1}^{n} a_i x_i$ for $x_i \in \mathbb{Z}_{\geq 0}$ for $i \in \{1, 2, ..., n\}$. In particular, $o_1 - 2$ cannot be expressed as a nonnegative integer linear combination of the a_i s. Thus, the Frobenius number F(a) is at least $o_1 - 2$, as required. \Box

The propositions outlined can be applied to establish a requirement for upper bounds on the Frobenius number, particularly where the weaker conditions (1) concerning the vector *a* are met.

Lemma 1. If an integer vector $\mathbf{a} = (a_1, a_2, ..., a_n)^T$ satisfies (1) with $a_1 \le a_2 \le \cdots \le a_n$, then any general upper bound on the Frobenius number $F(\mathbf{a})$ must inherently depend on the largest element a_n .

Proof. Let us suppose for simplicity that the vector a has the form that a_i is even for each $i \in \{1, 2, ..., n - 1\}$ while the final entry a_n is odd. Notice that here, $o_1 = a_n$ and, in light of Proposition 2, it immediately follows that $F(a) \ge a_n - 2$.

Suppose for contradiction that there exists an upper bound on F(a) that does not depend on a_n , i.e., that there exists some function $f : \mathbb{R}^{n-1} \to \mathbb{R}$ satisfying $F(a) \leq f(a_1, a_2, \ldots, a_{n-1})$. If we set $a_n = f(a_1, a_2, \ldots, a_{n-1}) + 3$ if $f(a_1, a_2, \ldots, a_{n-1})$ is even and $a_n = f(a_1, a_2, \ldots, a_{n-1}) + 4$ if $f(a_1, a_2, \ldots, a_{n-1})$ is odd, then we observe that $a_n - 2 > f(a_1, a_2, \ldots, a_{n-1})$ holds. In particular, notice that the lower bound on the Frobenius number is strictly larger than the (assumed) upper bound, which is a contradiction, as required. \Box

It should be emphasised that this result suggests that any (general) upper bound on the Frobenius number which does not depend on the maximal entry of a does not necessarily hold in general without stronger assumptions than the conditions in (1).

The following results provide a rather surprisingly useful property that holds when a satisfies the stronger conditions (2) that all the entries of the vector are pairwise coprime.

Lemma 2. If an integer vector $\mathbf{a} = (a_1, a_2, ..., a_n)^T$ satisfies (2), then for any $i, j \in \{1, 2, ..., n\}$ with $i \neq j$, we have

$$F(a) \leq (a_i - 1)(a_i - 1) - 1.$$

Proof. Firstly, notice that given any pair a_i and a_j with $i \neq j$, in light of the conditions in (2), it follows that $gcd(a_i, a_j) = 1$. Thus, the Frobenius number $F(a_i, a_j)$ corresponding to the pair a_i and a_j exists and takes a finite value. Furthermore, it follows, in light of (3), that the equality

$$F(a_i, a_i) = (a_i - 1)(a_i - 1) - 1$$

holds. By the definition of Frobenius number, we deduce that all integers strictly greater than $(a_i - 1)(a_j - 1) - 1$ can be expressed as $a_i x_i + a_j x_j$ for some $x_i, x_j \in \mathbb{Z}_{\geq 0}$. Thus, it immediately follows that all integers strictly greater than $(a_i - 1)(a_j - 1) - 1$ can be expressed as $\sum_{k=1}^{n} a_k x_k$ for $x_k \in \mathbb{Z}_{\geq 0}$ for $k \in \{1, 2, ..., n\}$ (upon setting $x_k = 0$ when $k \neq i, j$ whenever necessary). In particular, this shows that the Frobenius number F(a) satisfies the inequality $F(a) \leq (a_i - 1)(a_j - 1) - 1$ for any $i \neq j$, as required. \Box

The following corollary follows immediately from Lemma 2.

Corollary 1. If an integer vector $\mathbf{a} = (a_1, a_2, \dots, a_n)^T$ satisfies (2) and $a_1 \leq a_2 \leq \dots \leq a_n$, then

$$F(a) \le (a_1 - 1)(a_2 - 1) - 1.$$

It should be emphasised that the above results tell us that the well-known result (3) of Sylvester [11] extends naturally to provide an upper bound for the Frobenius number F(a) under the (stronger) assumption (2) that the entries of the vector a are pairwise coprime.

3. Observations on a Previously-Known Upper Bound

Recall that Beck et al. [15], Theorem 9 introduced the upper bound

$$F(a) \le \frac{1}{2} \left(\sqrt{a_1 a_2 a_3 (a_1 + a_2 + a_3)} - a_1 - a_2 - a_3 \right)$$
(4)

on the Frobenius number upon finding bounds for Fourier–Dedekind sums. This bound (4) is widely referenced across books and papers; however, in most of these, little attention is given to the underlying assumed conditions on a. In particular, the upper bound (4) necessitates that the stronger conditions (2) hold, instead of the more general (weaker) conditions (1).

Proposition 3. The upper bound (4) of Beck et al. [15], Theorem 9 does not necessarily hold unless the stronger conditions (2) hold. This requirement remains even if the weaker conditions (1) are met.

Proof. Observe that if n = 2, then the stronger (2) and weaker conditions (1) are equivalent. Thus, we focus here only on the case that $n \ge 3$, where we show that there are counterexamples for each n.

Let us consider two cases, namely n = 3 and $n \ge 4$, respectively. If n = 3, then consider the integer vector $\mathbf{a} = (3, 6, 19)^T$ with $F(\mathbf{a}) = 35$. In such case, notice that the bound (4) yields

$$\frac{1}{2}\left(\sqrt{3\cdot 6\cdot 19\left(3+6+19\right)}-3-6-19\right) = \frac{1}{2}\left(6\sqrt{266}-28\right) \approx 34.928519\tag{5}$$

where, in particular, $35 \leq 34.928519$ and, hence, the upper bound (4) fails when n = 3. If, instead, $n \geq 4$, then in light of Lemma 1, clearly (4) cannot be a general upper bound for the Frobenius number. \Box

Note that in the case of $n \ge 4$, any vector $a = (2, 4, 6, a_4, ..., a_n)^T$ satisfying (1) and $a_n \ge \cdots \ge a_4 > 7$ provides a counterexample for any n. Indeed, since $a_4 > 7$ by assumption, the Frobenius number is clearly greater than or equal to 7 (since 7 cannot be expressed by $\sum_{i=1}^{n} a_i x_i$ for $x_i \in \mathbb{Z}_{\ge 0}$ for all i). Despite this, the bound (4) yields

$$\frac{1}{2}\left(\sqrt{2\cdot 4\cdot 6\left(2+4+6\right)}-2-4-6\right)=6,$$
(6)

which demonstrates that the upper bound (4) does not necessarily hold if only the weaker conditions (1) are met.

The remarks presented in this section are intended to clarify a common misunderstanding about the upper bound (4) as referenced in various books and papers. Furthermore, it is crucial to highlight a subtle error in the argument presented by Beck et al. [15], which alters the value of the upper bound. The following result states the corrected upper bound, where the proof is outlined in a later section.

Theorem 1. If an integer vector $\mathbf{a} = (a_1, a_2, ..., a_n)^T$ satisfies (2) with $a_1 \le a_2 \le \cdots \le a_n$, then the argument of Beck et al. [15] yields

$$F(a) \leq \frac{1}{2} \left(\sqrt{\frac{1}{3}(a_1 + a_2 + a_3)(a_1 + a_2 + a_3 + 2a_1a_2a_3) + \frac{8}{3}(a_1a_2 + a_2a_3 + a_3a_1)} - a_1 - a_2 - a_3 \right).$$
(7)

It is natural to consider if the original bound (4) given by Beck et al. [15], Theorem 9 is indeed correct provided that the integer vector a satisfies the stronger conditions (2). It turns out that the upper bound (4) remains valid. The following result states this formally, where the proof is outlined in a later section.

Theorem 2. If an integer vector $\mathbf{a} = (a_1, a_2, \dots, a_n)^T$ satisfies (2) with $a_1 \le a_2 \le \dots \le a_n$, then

$$F(\mathbf{a}) \leq \frac{1}{2} \left(\sqrt{a_1 a_2 a_3 (a_1 + a_2 + a_3)} - a_1 - a_2 - a_3 \right).$$

Furthermore, it is natural to consider the relative tightness of (1) with (4). This comparison will be explored in the subsequent section of the paper.

4. Tightness Comparison of Upper Bounds

In this section, we consider the relative tightness of the upper bounds (1) and (4). In particular, to slightly simplify notation, let us denote by

$$UB_{1}(a) = UB_{1}(a_{1}, a_{2}, a_{3})$$

$$:= \frac{1}{2} \left(\sqrt{\frac{1}{3}(a_{1} + a_{2} + a_{3})(a_{1} + a_{2} + a_{3} + 2a_{1}a_{2}a_{3}) + \frac{8}{3}(a_{1}a_{2} + a_{2}a_{3} + a_{3}a_{1})} - a_{1} - a_{2} - a_{3} \right)$$

and

$$UB_2(a) = UB_2(a_1, a_2, a_3) := \frac{1}{2} \left(\sqrt{a_1 a_2 a_3 (a_1 + a_2 + a_3)} - a_1 - a_2 - a_3 \right).$$

Recall that Theorem 1 and 2 imply that $UB_1(a)$ and $UB_2(a)$ are valid upper bounds provided that a satisfies (2) and $a_1 \le a_2 \le \cdots \le a_n$; however, we are instead interested in which bound is tighter. The first result of this section shows that $UB_2(a)$ is tighter than $UB_1(a)$ in only a relatively "small" (finite) number of cases, where the proof is excluded, given that this was completed via simple enumeration.

Theorem 3. If an integer vector $\mathbf{a} = (a_1, a_2, ..., a_n)^T$ satisfies (2) with $a_1 \le a_2 \le \cdots \le a_n$, then $F(\mathbf{a})$ satisfies $F(\mathbf{a}) \le UB_1(\mathbf{a})$ and $F(\mathbf{a}) \le UB_2(\mathbf{a})$, where $UB_2(\mathbf{a})$ is sharper only when

 $\begin{aligned} (a_1, a_2, a_3) &\in \big\{ (1, 2, 3), (1, 2, 5), (1, 2, 7), (1, 2, 9), (1, 2, 11), (1, 2, 13), (1, 2, 15), \\ &\quad (1, 2, 17), (1, 2, 19), (1, 2, 21), (1, 2, 23), (1, 2, 25), (1, 3, 4), (1, 3, 5), \\ &\quad (1, 3, 7), (1, 3, 8), (1, 3, 10), (1, 3, 11), (1, 3, 13), (1, 3, 14), (1, 4, 5), \\ &\quad (1, 4, 7), (1, 4, 9), (1, 4, 11), (1, 5, 6), (1, 5, 7), (1, 5, 8), (1, 5, 9), (1, 6, 7), (2, 3, 5) \big\}. \end{aligned}$

It should be emphasised that this result suggests that in "almost all" cases, $UB_1(a)$ provides a tighter bound than $UB_2(a)$. Note that in the above, we assume the stronger conditions (2) rather than the weaker conditions (1) since the examples (5) and (6) show that $UB_1(a)$ and $UB_2(a)$ do not necessarily apply under only (1). In order to compare the relative tightness of the bounds, for completeness, we applied Monte Carlo simulation techniques (see, e.g., [35] [Chapter 2]) and present the results below.

During this simulation, we firstly randomly generated integer vectors a satisfying the conditions (2) with the ordering $a_1 \le a_2 \le \cdots \le a_n$ before computing the values of $UB_1(a)$ and $UB_2(a)$. This process was iteratively repeated 100,000 times. During the sampling, we set $||a||_{\infty} = \max_i |a_i| \le 1000$ for convenience. Note that in each graph in Figure 1, the vertical axis corresponds to the difference $UB_1(a) - UB_2(a)$, where a large vertical value illustrates that the corrected upper bound (7) is much tighter than the originally stated bound (4).

Figure 1a demonstrates that the difference $UB_1(a) - UB_2(a)$ grows rapidly with increases in a_3 , while the difference remains small if a_3 is small. It should be emphasised that one would not expect the difference to be significant when a_3 is small given that the entries of a are ordered by assumption. Figure 1b shows how this differences varies upon increases in a_1a_2 . Notably, the figure suggests that the minimum difference increases linearly with a_1a_2 , whereas the maximum difference seems to grow sublinearly with a_1a_2 . Furthermore, if a_1a_2 is large (around 1,000,000), then the variance of the difference $UB_1(a) - UB_2(a)$ appears small. This can be explained by considering the difference

$$UB_{1}(a) - UB_{2}(a) = \frac{1}{2} \Big(\sqrt{a_{1}a_{2}a_{3}(a_{1} + a_{2} + a_{3})} - \sqrt{\frac{1}{3}a_{1}a_{2}a_{3}(a_{1} + a_{2} + a_{3}) + (a_{1} + a_{2} + a_{3})^{2} + \frac{8}{3}(a_{1}a_{2} + a_{2}a_{3} + a_{3}a_{1})} \Big),$$

which is maximised for fixed a_1a_2 when a_3 is large and is minimised when a_3 is small. In particular, note that if a_3 is small, then the assumed ordering implies that $a_3 \approx a_2$. In such case, the value of the difference can be well approximated by

$$\frac{1}{2}a_1a_2\left(\sqrt{3}-\sqrt{2+\frac{11}{a_1a_2}}\right),$$

which grows roughly linearly. If, instead, a_1a_2 is large (say around 1,000,000), then the assumed ordering and upper bound on the a_i s restricts variance in both $UB_1(a)$ and $UB_2(a)$, respectively. Figure 1c demonstrates that the difference $UB_1(a) - UB_2(a)$ grows sublinearly with the product $a_1a_2a_3$, while the variance once more appears small, which can be similarly explained via careful algebraic analysis. Figure 1d shows how this difference varies upon increases in $a_1 + a_2 + a_3$, where the variance decreases significantly as the value of $a_1 + a_2 + a_3$ grows beyond 2000. Notably, the final figure suggests that one should expect



the difference $UB_1(a) - UB_2(a)$ to be small only in the scenario that a_1 is "reasonably small", which follows in light of the assumed ordering.

Figure 1. This figure illustrates how the difference $UB_1(a) - UB_2(a)$ varies dependently upon the a_i s. (a) $UB_1(a) - UB_2(a)$ upon increasing the entry a_3 . (b) $UB_1(a) - UB_2(a)$ upon increasing the product a_1a_2 . (c) $UB_1(a) - UB_2(a)$ upon increasing the product $a_1a_2a_3$. (d) $UB_1(a) - UB_2(a)$ upon increasing the sum $a_1 + a_2 + a_3$.

5. Proof of Theorem 1

In this section, we follow closely the argument presented by Beck et al. [15] [Theorem 9] to demonstrate that it actually yields the upper bound (7) instead of (4). It should be noted that the proof presented by Beck et al. [15] instead provides an upper bound for

$$F^*(\boldsymbol{a}) := \max\left\{b \in \mathbb{Z} : b \neq \boldsymbol{a}^T \boldsymbol{z} \text{ for all } \boldsymbol{z} \in \mathbb{Z}_{>0}^n\right\}$$
$$= F(\boldsymbol{a}) + a_1 + a_2 + \dots + a_n,$$

which is the largest integer that cannot be represented as a (strictly) positive integer combination of the a_i s.

Let $A = \{a_1, a_2, ..., a_n\}$ be a set of pairwise coprime positive integers and define the function

$$p'_{A}(b) = \#\left\{ (m_{1}, \dots, m_{n})^{T} \in \mathbb{Z}_{>0}^{n} : \sum_{k=1}^{n} m_{k} a_{k} = b \right\},\$$

where # denotes the cardinality of the set. Specifically, $p'_A(b)$ counts the number of (strictly) positive tuples $(m_1, \ldots, m_n)^T \in \mathbb{Z}_{>0}^n$ satisfying the equality $\sum_{k=1}^n m_k a_k = b$. Notice that $F^*(a)$ is simply the largest value for *b* for which $p'_A(b) = 0$.

Let $c_1, c_2, \ldots, c_n \in \mathbb{Z}$ be relatively prime to $c \in \mathbb{Z}$, and $t \in \mathbb{Z}$. We define the Fourier–Dedekind sum as

$$\sigma_t(c_1,\ldots,c_n;c)=\frac{1}{c}\sum_{\lambda^c=1\neq\lambda}\frac{\lambda^t}{(\lambda^{c_1}-1)\cdots(\lambda^{c_n}-1)}.$$

Note that one particularly noteworthy expression (which is followed by periodicity) [15] is

$$\sigma_t(a,b;c) = \sum_{m=0}^{c-1} \left(\left(\frac{-a^{-1}(bm+t)}{c} \right) \right) \left(\left(\frac{m}{c} \right) \right) - \frac{1}{4c}$$
(8)

with $aa^{-1} \equiv 1 \pmod{c}$ and where $((x)) = x - \lfloor x \rfloor - \frac{1}{2}$ is a sawtooth function.

Proof. Firstly, note that it is easy to verify that

$$F^*(a) = F^*(a_1, a_2, \dots, a_n) \le F^*(a_1, a_2, a_3) + a_3 + a_4 + \dots + a_n$$

We closely follow [15] by focusing on the case where n = 3 and the a_i s are pairwise coprime. In order to slightly simplify notation, let a, b, c denote pairwise relatively prime positive integers. Upon using the the Cauchy–Schwartz inequality, we find that

$$\sigma_t(a,b;c) \ge -\sum_{m=0}^{c-1} \left(\left(\frac{m}{c}\right) \right)^2 - \frac{1}{4c} = \sum_{m=0}^{c-1} \left(\frac{m}{c} - \frac{1}{2}\right)^2 - \frac{1}{4c}$$
$$= -\frac{1(2c-1)(c-1)c}{c^2} + \frac{1}{c}\frac{c(c-1)}{2} - \frac{c}{4} - \frac{1}{4c}$$
$$= -\frac{c}{12} - \frac{5}{12c}.$$

It should be noted that in [15], the right-hand side of the expression previously discussed differs from the one presented here. We can now utilise the above inequality to obtain

$$\begin{split} p'_{\{a,b,c\}}(t) &\geq \frac{t^2}{2abc} - \frac{t}{2} \left(\frac{1}{ab} + \frac{1}{ac} + \frac{1}{bc} \right) + \frac{1}{12} \left(\frac{3}{a} + \frac{3}{b} + \frac{3}{c} + \frac{a}{bc} + \frac{b}{ac} + \frac{c}{ab} \right) \\ &- \frac{1}{12} (a + b + c) - \frac{5}{12} \left(\frac{1}{a} + \frac{1}{b} + \frac{1}{c} \right) \\ &= \frac{t^2}{2abc} - \frac{t}{2} \left(\frac{1}{ab} + \frac{1}{ac} + \frac{1}{bc} \right) + \frac{1}{12} \left(\frac{a}{bc} + \frac{b}{ac} + \frac{c}{ab} \right) \\ &- \frac{1}{12} (a + b + c) - \frac{1}{6} \left(\frac{1}{a} + \frac{1}{b} + \frac{1}{c} \right), \end{split}$$

which, upon algebraic manipulation, yields the upper bound

$$F^*(a,b,c) \le \frac{1}{2}(a+b+c) + \frac{1}{2}\sqrt{\frac{1}{3}(a+b+c)(a+b+c+2abc) + \frac{8}{3}(ab+bc+ca)}$$

Thus, upon replacing a, b and c with a_1 , a_2 and a_3 , respectively, we deduce that

$$F^{*}(a) \leq F^{*}(a_{1}, a_{2}, a_{3}) + a_{3} + a_{4} + \dots + a_{n}$$

$$\leq \left(\frac{1}{2}\sqrt{\frac{1}{3}(a_{1} + a_{2} + a_{3})(a_{1} + a_{2} + a_{3} + 2a_{1}a_{2}a_{3}) + \frac{8}{3}(a_{1}a_{2} + a_{2}a_{3} + a_{3}a_{1})} + a_{1} + a_{2} + a_{3}\right)$$

$$+ a_{3} + a_{4} + \dots + a_{n}$$

which yields that

$$F(a) = F^*(a) - a_1 - a_2 - \dots - a_n$$

$$\leq \frac{1}{2} \left(\sqrt{\frac{1}{3}(a_1 + a_2 + a_3)(a_1 + a_2 + a_3 + 2a_1a_2a_3) + \frac{8}{3}(a_1a_2 + a_2a_3 + a_3a_1)} - a_1 - a_2 - a_3 \right)$$

as required, which concludes the proof. \Box

6. Proof of Theorem 2

Recall the notation

$$UB_{1}(a) := \frac{1}{2} \left(\sqrt{\frac{1}{3} (a_{1} + a_{2} + a_{3}) (a_{1} + a_{2} + a_{3} + 2a_{1}a_{2}a_{3}) + \frac{8}{3} (a_{1}a_{2} + a_{2}a_{3} + a_{3}a_{1})} - a_{1} - a_{2} - a_{3} \right)$$

and

$$UB_2(a) := \frac{1}{2} \left(\sqrt{a_1 a_2 a_3 (a_1 + a_2 + a_3)} - a_1 - a_2 - a_3 \right)$$

In this section, we show that $UB_2(a)$ is a valid upper bound on the Frobenius number F(a) provided a satisfies (2) and $a_1 \le a_2 \le \cdots \le a_n$. It should be noted that the stronger condition (2) with the (assumed) ordering of the a_i s implies that $a_1 < a_2 < \cdots < a_n$, provided that $a_1 > 1$. Before discussing the correctness of the upper bound $UB_2(a)$, we firstly consider how this bound varies with changes in a_3 .

Proposition 4. If $a_1 < a_2 < a_3$, then $UB_2(a)$ is a strictly increasing function in a_3 . If, instead, $a_1 \le a_2 \le a_3$ holds, then $UB_2(a)$ is a nondecreasing function in a_3 .

Proof. Upon partial differentiation with respect to a_3 , observe that $UB_2(a)$ becomes

$$\frac{\partial UB_2(a)}{\partial a_3} = \frac{1}{2} \left(\frac{a_1 a_2(a_1 + a_2 + 2a_3)}{2\sqrt{a_1 a_2 a_3(a_1 + a_2 + a_3)}} - 1 \right).$$

If $a_1 < a_2 < a_3$, then note that $a_1a_2(a_1 + a_2 + 2a_3) > 4a_3$ holds. Upon simple algebraic manipulation, we deduce that $a_1^2a_2^2(a_1 + a_2 + 2a_3)^2 > 4a_1a_2a_3(a_1 + a_2 + a_3)$, which implies that

$$\frac{a_1a_2(a_1+a_2+2a_3)}{2\sqrt{a_1a_2a_3(a_1+a_2+a_3)}} > 1.$$

It follows that $\frac{\partial UB_2(a)}{\partial a_3} > 0$ and, hence, $UB_2(a)$ is a strictly increasing function in a_3 when $a_1 < a_2 < a_3$. If, instead, $a_1 \le a_2 \le a_3$, then a similar argument yields that $\frac{\partial UB_2(a)}{\partial a_3} \ge 0$ and, hence, $UB_2(a)$ is a nondecreasing function in a_3 , as required. \Box

We now proceed to present a detailed proof to establish the validity of Theorem 2.

Proof. Observe that if $UB_2(a) \ge UB_1(a)$, then clearly the upper bound $UB_2(a)$ is valid in consequence to the validity of Theorem 1. Thus, we consider only the setting where $UB_2(a) < UB_1(a)$. Notice that upon simple algebraic manipulation, the inequality $UB_2(a) \le UB_1(a)$ is equivalent to

$$a_1a_2a_3(a_1+a_2+a_3) \le a_1^2 + a_2^2 + a_3^2 + 10(a_1a_2+a_2a_3+a_1a_3).$$
(9)

It is sufficient to here consider only the case that $a_1 < a_2 < a_3$. In particular, this follows because otherwise we require $a_1 = 1$ in light of the assumed conditions in (2), and hence, in such case, we yield that $F(a) = -1 \le UB_2(a)$ holds, as required.

In order to satisfy (9), the (strict) inequality $a_1a_2 < 33$ is necessary. Indeed, if instead $a_1a_2 \ge 33$, then

$$\begin{aligned} a_1 a_2 a_3 (a_1 + a_2 + a_3) &= a_1 a_2 a_3^2 + a_1 a_2 a_3 (a_1 + a_2) \\ &> a_1 a_2 a_3^2 \\ &\ge 33 a_3^2 \\ &= 3a_3^2 + 10(a_3^2 + a_3^2 + a_3^2) \\ &> a_1^2 + a_2^2 + a_3^2 + 10(a_1 a_2 + a_2 a_3 + a_1 a_3) \end{aligned}$$

holds, where the final inequality follows since $a_1, a_2 < a_3$. Thus, we need only to consider the cases that $a_1a_2 \leq 32$ and $a_1 < a_2$ with $gcd(a_1, a_2) = 1$. The pairs (a_1, a_2) satisfying these conditions are as follows:

- 1. if $a_1 = 1$, then $(a_1, a_2) = (1, 2), (1, 3), \dots, (1, 31), (1, 32);$
- 2. if $a_1 = 2$, then $(a_1, a_2) = (2, 3), (2, 5), (2, 7), (2, 9), (2, 11), (2, 13), (2, 15);$
- 3. if $a_1 = 3$, then $(a_1, a_2) = (3, 4), (3, 5), (3, 7), (3, 8), (3, 10);$
- 4. if $a_1 = 4$, then $(a_1, a_2) = (4, 5), (4, 7);$
- 5. if $a_1 = 5$, then $(a_1, a_2) = (5, 6)$.

It should be emphasised that if $UB_2(a)$ is a valid upper bound in each of the above cases, then it follows that $UB_2(a)$ is a valid upper bound, as required. In order to complete the proof, we now consider each of these cases in turn. It should be noted that cases (ii)–(v) use the properties $F(a) \le (a_1 - 1)(a_2 - 1) - 1$ (which follows Corollary 1) and $UB(a_1, a_2, a'_3) > UB(a_1, a_2, a_3)$ when $a'_3 > a_3$ (which follows Proposition 4).

1. $a_1 = 1$: In this case, notice that since the entries of the vector a are coprime by assumption, it follows that we have $a_2 \ge 2$ and $a_3 \ge 3$. Note that we have $(a_2 - 1)(a_3 - 1) \ge 2$ and $a_2a_3 \ge 1 + a_2 + a_3$. These inequalities imply that

$$a_2a_3(1+a_2+a_3) \ge (1+a_2+a_3)^2$$

which, upon rearranging algebraically, yields that

$$\frac{1}{2}\left(\sqrt{a_2a_3(1+a_2+a_3)}-(1+a_2+a_3)\right)=UB_2(1,a_2,a_3,\ldots,a_n)\geq 0.$$

Finally, observe that the equality $F(1, a_2, a_3, ..., a_n) = -1$ holds for all $a_2, a_3, ..., a_n$ and, thus, $UB_2(a)$ is a valid upper bound in this scenario.

2. $a_1 = 2$: In this case, notice that

$$F(2,3,a_3,a_4,\ldots,a_n) \le (2-1)(3-1) - 1 = 1 < 3.660254 = UB_2(2,3,5) \le UB_2(2,3,5)$$

where the strict inequality follows since if $(a_1, a_2) = (2, 3)$, then $a_3 \ge 5$ by the conditions (2). In a similar fashion, notice that

$$F(2,5,a_3,a_4,\ldots,a_n) \le (2-1)(5-1) - 1 = 3 < 8.652476 = UB_2(2,5,7) \le UB_2(2,5,a_3),$$

$$F(2,7,a_3,a_4,\ldots,a_n) \le (2-1)(7-1) - 1 = 5 < 14.811762 = UB_2(2,7,9) \le UB_2(2,7,a_3),$$

 $\begin{aligned} F(2,9,a_3,a_4,\ldots,a_n) &\leq (2-1)(9-1) - 1 = 7 < 22 = UB_2(2,9,11) \leq UB_2(2,9,a_3), \\ F(2,11,a_3,a_4,\ldots,a_n) &\leq (2-1)(11-1) - 1 = 9 < 30.116122 \\ &= UB_2(2,11,13) \leq UB_2(2,11,a_3), \\ F(2,13,a_3,a_4,\ldots,a_n) &\leq (2-1)(13-1) - 1 = 11 < 39.083269 \\ &= UB_2(2,13,15) \leq UB_2(2,13,a_3), \end{aligned}$

$$F(2, 15, a_3, a_4, \dots, a_n) \le (2-1)(15-1) - 1 = 13 < 48.8407169$$

= $UB_2(2, 15, 17) \le UB_2(2, 15, a3)$.

3. $a_1 = 3$: In this case, notice that

$$\begin{split} F(3,4,a_3,a_4,\ldots,a_n) &\leq (3-1)(4-1) - 1 = 5 < 7.416408 = UB_2(3,4,5) \leq UB_2(3,4,a_3), \\ F(3,5,a_3,a_4,\ldots,a_n) &\leq (3-1)(5-1) - 1 = 9 < 12.343135 = UB_2(3,5,7) \leq UB_2(3,5,a_3), \\ F(3,7,a_3,a_4,\ldots,a_n) &\leq (3-1)(7-1) - 1 = 11 < 18.495454 = UB_2(3,7,8) \leq UB_2(3,7,a_3), \\ F(3,8,a_3,a_4,\ldots,a_n) &\leq (3-1)(8-1) - 1 = 13 < 27.105118 = UB_2(3,8,11) \leq UB_2(3,8,a_3), \end{split}$$

$$F(3, 10, a_3, a_4, \dots, a_n) \le (3-1)(10-1) - 1 = 17 < 32.497191$$

= $UB_2(3, 10, 11) \le UB_2(3, 10, a_3).$

4. $a_1 = 4$: In this case, notice that

 $F(4,5,a_3,a_4,\ldots,a_n) \le (4-1)(5-1) - 1 = 11 < 15.6643191 = UB_2(4,5,7) \le UB_2(4,5,a_3),$

- $F(4,7,a_3,a_4,\ldots,a_n) \le (4-1)(7-1) 1 = 17 < 25.496479 = UB_2(4,7,9) \le UB_2(4,7,a_3).$
- 5. $a_1 = 5$: In this case, notice that

$$F(5, 6, a_3, a_4, \dots, a_n) \le (5-1)(6-1) - 1 = 19 < 21.740852 = UB_2(5, 6, 7) \le UB_2(5, 6, a_3).$$

Thus, provided that $a_1a_2 \leq 32$, then $F(a) < UB_2(a_1, a_2, a_3) = UB_2(a)$. Thus, it follows that $UB_2(a)$ is indeed a valid upper bound in all cases, which concludes the proof. \Box

7. Conclusions and Future Work

In this paper, we revisited the classical Frobenius problem and examined a previously established upper bound on the Frobenius number. Our analysis revealed a subtle error in the original argument of Beck et al. [15], Theorem 9, leading to a revised and corrected upper bound. While this error did not invalidate the bound itself, it impacted its tightness. We also compared the relative tightness of the original and corrected bound through theoretical analysis and Monte Carlo simulations, demonstrating that the corrected bound is tighter in all but a relatively "small" (finite) number of cases.

This study opens several rather promising avenues for future research. Firstly, a case-specific analysis could explore the behavior and tightness of upper bounds under different assumptions around the distribution of the input vector a, such as uniform or exponential distributions. This would provide deeper insights into how the nature of the input impacts upon the bounds' performance. Secondly, exploring the applications of these bounds in optimisation problems, particularly in knapsack or subset–sum problems, would be valuable. Understanding particularly how these bounds influence computational efficiency and solution "quality" in real-world settings could significantly broaden their utility. Finally, the further examination of the geometric properties of the knapsack polytope P(a, b) associated with the Frobenius problem may uncover deeper connections between geometric insights and the derivation of (perhaps) sharper upper bounds, particularly in higher-dimensional scenarios or under additional assumptions.

Author Contributions: All authors contributed equally to the research. All authors have read and agreed to the published version of the manuscript.

Funding: This research received no external funding.

Data Availability Statement: The original contributions presented in the study are included in the article, further inquiries can be directed to the corresponding author.

Conflicts of Interest: The authors declare no conflicts of interest.

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