Lagrange's Theorem for Binary Squares

P. Madhusudan¹

Department of Computer Science, Thomas M. Siebel Center for Computer Science, 201 North Goodwin Avenue, Urbana, IL 61801-2302, USA madhu@illinois.edu

https://orcid.org/0000-0002-9782-721X

Dirk Nowotka

Department of Computer Science, Kiel University, D-24098 Kiel, Germany dn@informatik.uni-kiel.de

https://orcid.org/0000-0002-5422-2229

Aayush Rajasekaran

School of Computer Science, University of Waterloo, Waterloo, ON N2L 3G1, Canada arajasekaran@uwaterloo.ca

Jeffrey Shallit

School of Computer Science, University of Waterloo, Waterloo, ON N2L 3G1, Canada shallit@uwaterloo.ca

(b) https://orcid.org/0000-0003-1197-3820

Abstract -

We show how to prove theorems in additive number theory using a decision procedure based on finite automata. Among other things, we obtain the following analogue of Lagrange's theorem: every natural number > 686 is the sum of at most 4 natural numbers whose canonical base-2 representation is a binary square, that is, a string of the form xx for some block of bits x. Here the number 4 is optimal. While we cannot embed this theorem itself in a decidable theory, we show that stronger lemmas that imply the theorem can be embedded in decidable theories, and show how automated methods can be used to search for these stronger lemmas.

2012 ACM Subject Classification Theory of computation \rightarrow Models of computation, Theory of computation \rightarrow Constructive mathematics, Mathematics of computing \rightarrow Discrete mathematics

Keywords and phrases binary square, theorem-proving, finite automaton, decision procedure, decidable theory, additive number theory

Digital Object Identifier 10.4230/LIPIcs.MFCS.2018.18

1 Introduction

Additive number theory is the study of the additive properties of integers [12]. In particular, an additive basis of order h is a subset $S \subseteq \mathbb{N}$ such that every natural number is the sum of h members, not necessarily distinct, of S. The principal problem of additive number theory is to determine whether a given subset S is an additive basis of order h for some h, and if so, to determine the smallest value of h. There has been much research in the area, and deep techniques, such as the Hardy-Littlewood circle method, have been developed to solve these kinds of problems [20].

One of the earliest results in additive number theory is Lagrange's famous theorem [10] that every natural number is the sum of four squares [5, 11]. In the terminology of

 $^{^{1}}$ This material is based upon work supported by the National Science Foundation under Grant No. 1527395.

the previous paragraph, this means that $S = \{0^2, 1^2, 2^2, 3^2, \ldots\}$ forms an additive basis of order 4. The celebrated problem of Waring (1770) (see, e.g., [4, 19, 21]) is to determine the corresponding least order g(k) for k'th powers. Since it is easy to see that numbers of the form $4^a(8k+7)$ cannot be expressed as the sum of three squares, it follows that g(2) = 4. It is known that g(3) = 9 and g(4) = 19.

In a variation on this concept we say that $S \subseteq \mathbb{N}$ is an asymptotic additive basis of order h if every sufficiently large natural number is the sum of h members, not necessarily distinct, of S. The classical function G(k) is defined to be the least asymptotic basis order for k'th powers. From above we have G(2) = 4. It is known that G(14) = 16, and $4 \le G(3) \le 7$. Despite much work, the exact value of G(3) is currently unknown.

Recently there has been interest in doing additive number theory on sets of natural numbers whose base-k representations have certain properties. For example, Banks [1] proved that every natural number is the sum of at most 49 natural numbers whose decimal representation is a palindrome. This was improved by Cilleruelo, Luca, and Baxter [2] to 3 summands for every base $b \geq 5$. The remaining cases b = 2, 3, 4 were recently resolved [17].

In this paper we consider a variation on Lagrange's theorem. Instead of the ordinary notion of the square of an integer, we consider "squares" in the sense of formal language theory [8]. That is, we consider x, the canonical binary (base-2) representation of an integer N, and call N a binary square if N=0, or if x=yy for some nonempty string y that starts with a 1. Thus, for example, N=221 is a binary square, since 221 in base 2 is 11011101=(1101)(1101). The first few binary squares are

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0, 3, 10, 15, 36, 45, 54, 63, 136, 153, 170, 187, 204, 221, 238, 255, \dots;
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they form sequence <u>A020330</u> in the *On-Line Encyclopedia of Integer Sequences* (OEIS) [18]. Clearly a number N>0 is a binary square if and only if it is of the form $a(2^n+1)$ for $n\geq 1$ and $2^{n-1}\leq a<2^n$. This is a very natural sequence to study, since the binary squares have density $\Theta(N^{1/2})$ in the natural numbers, just like the ordinary squares. (There exist sets of density $\Theta(N^{1/2})$ that do not form an asymptotic basis of finite order, so density considerations alone do *not* imply our result.)

In this paper we prove the following result.

▶ **Theorem 1.** The binary squares form an asymptotic basis of order 4. More precisely, every natural number N > 686 is the sum of 4 binary squares. There are 56 exceptions, given below:

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1, 2, 4, 5, 7, 8, 11, 14, 17, 22, 27, 29, 32, 34, 37, 41, 44, 47, 53, 62, 95, 104, 107, 113, 116, 122, 125, \\131, 134, 140, 143, 148, 155, 158, 160, 167, 407, 424, 441, 458, 475, 492, 509, 526, 552, 560, \\569, 587, 599, 608, 613, 620, 638, 653, 671, 686.
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The novelty in our approach is that we obtain this theorem in additive number theory using very little number theory at all. Instead, we use an approach based on formal language theory, reducing the proof of the theorem to a decidable language emptiness problem. Previously we obtained similar results for palindromes [15, 16, 17].

1.1 Search for appropriate lemmas and proving the theorem

The technique we use for encoding Theorem 1 as a problem dealing with automata is to ask, for all sufficiently large integers N, whether there exist four binary squares with representation $x_i x_i$, $1 \le i \le 4$, such that the sum of the numbers they represent is N. Since the language of

binary squares is not regular, we use an encoding where we represent only one copy of each x_i and reuse it to represent the number. However, it turns out that we cannot represent the desired theorem directly as an emptiness/universality problem of finite automata. The reason is that when representing only one copy of the x_i , we can do "school addition" (aligning them and adding the numbers, columnwise, with a carry) only if the words x_i are roughly of the same *length*. More precisely, we require the lengths of the squares employed to either be bounded by a constant, or differ from each other and from the number N only by a bounded length.

For fixed constants k_i , $1 \le i \le 4$, we observe that the set of all binary representations of N for which there exist four words x_i , $1 \le i \le 4$, of lengths $L - k_i$, such that the binary representation of N is of length 2L and the sum of the numbers represented by x_ix_i , $1 \le i \le 4$ is N, is a regular language. Thus we can prove, using known decision algorithms for automata, lemmas that assert that all numbers of a particular form can be represented by a sum of four binary squares, where the binary squares are of various lengths $L - k_1$, $L - k_2$, $L - k_3$, and $L - k_4$, for a finite set of tuples $\langle k_1, k_2, k_3, k_4 \rangle$ (see Lemma 5 for such a lemma).

Proving such a lemma for a particular set of combinations of lengths implies the theorem, of course, but the lemma itself is stronger. The truth of such stronger lemmas is decidable, while we don't have a way to directly decide the theorem itself!

Thus we need a *search* for an appropriate lemma for a particular combination of length differences that is valid. Given that checking these lemmas for any set of combinations is decidable, we can do the search for these lemmas automatically. We tried various combinations and succeeded in proving one lemma, namely Lemma 5, that implies our theorem.

The above technique can be generalized to some extent – evidently, we could also consider the analogous results for other powers such as cubes, and bases $b \ge 2$, but we do not do that in this paper.

1.2 Notation

We are concerned with the binary representation of numbers, so let us introduce some notation. If N is a natural number, then by $(N)_2$ we mean the string giving the canonical base-2 representation of N, having no leading zeroes. For example, $(43)_2 = 101011$. The canonical representation of 0 is ϵ , the empty string.

If $2^{n-1} \le N < 2^n$ for $n \ge 1$, we say that N is an n-bit integer in base 2. Note that the first bit of the binary representation of an n-bit integer is always nonzero. The length of an integer N satisfying $2^{n-1} \le N < 2^n$ is defined to be n; alternatively, the length of N is $1 + \lfloor \log_2 N \rfloor$. For $n \ge 1$ we define $C_n = \{a \cdot (2^n + 1) : 2^{n-1} \le a < 2^n\}$, the set of all 2n-bit binary squares.

2 A classical approach

In this section we describe how one can apply classical number-theoretic and combinatorial tools to this problem to obtain some results weaker than Theorem 1. The idea is to show that the numbers that are the sum of two binary squares form a set of positive lower asymptotic density. (In contrast, our approach via automata, which we discuss in later sections, provides more precise results.)

For sets $S, T \subseteq \mathbb{N}$ we define the sumset $S + T = \{s + t : s \in S, t \in T\}$. The cardinality of a finite set S is denoted by |S|. Given a set $S \subseteq \mathbb{N}$, the lower asymptotic density of S is defined to be

$$d(S) = \liminf_{n \to \infty} \frac{|\{x \in S \ : \ 1 \le x \le n\}|}{n}.$$

We first prove

▶ **Lemma 2.** For $n \ge 1$ we have $|C_n + C_{n+1}| = 2^{2n-1}$.

Proof. Since $|C_n| = 2^{n-1}$ and $|C_{n+1}| = 2^n$, this lemma is equivalent to the claim that each member of the sumset $C_n + C_{n+1}$ has a *unique* representation as the sum of one element of C_n and one element of C_{n+1} .

We argue by contradiction. Suppose the representation is not unique, and there exist integers a, a' with $2^{n-1} \le a, a' < 2^n - 1$ and integers b, b' with $2^n \le b, b' < 2^{n+1}$ such that $(a, a') \ne (b, b')$ but

$$a \cdot (2^{n} + 1) + b \cdot (2^{n+1} + 1) = a' \cdot (2^{n} + 1) + b' \cdot (2^{n+1} + 1). \tag{1}$$

Computing Eq. (1) modulo $2^n + 1$, we see that $-b \equiv -b' \pmod{2^n + 1}$. Since $2^n \leq b, b' < 2^{n+1}$ we see the congruence in fact implies that b = b'. But then a = a', a contradiction.

▶ **Theorem 3.** The numbers that are the sum of two binary squares form a set of lower asymptotic density $\geq 1/40$.

Proof. Let S_2 be the set of numbers that are the sum of two binary squares. Clearly $C_n + C_{n+1} \subseteq S_2$.

There are 2^{2n-1} elements in the sumset $C_n + C_{n+1}$, whose largest element is $(2^n - 1)2^n + (2^{n+1} - 1)2^{n+1} = 5 \cdot 2^{2n} - 3 \cdot 2^n$. Given an integer $m \ge 14$, choose $n \ge 1$ such that $5 \cdot 2^{2n} - 3 \cdot 2^n < m < 5 \cdot 2^{2n+2} - 3 \cdot 2^{n+1}$. Then

$$\frac{\left|\{x \in S_2 \ : \ 1 \le x \le m\}\right|}{m} \ge \frac{2^{2n-1}}{5 \cdot 2^{2n+2}} = \frac{1}{40}.$$

▶ Corollary 4. The binary squares form an asymptotic basis of finite order.

Proof. This is a direct consequence of a result of Nathanson [13, Theorem 11.6, p. 366], which says that if a subset S of \mathbb{N} has $0 \in S$, gcd(S) = 1, and has positive lower asymptotic density, then it is an asymptotic basis of finite order. It is now easy to check that the hypotheses are fulfilled for $S = S_2$.

▶ Remark. It would be interesting to determine the exact lower asymptotic density of the set S_2 . Numerical computation suggests that perhaps $d(S_2) \doteq .14$.

The automaton approach: the main lemma

Now we turn to a completely different approach to the theorem for binary squares, as sketched in Section 1, using automata theory. This allows us to obtain the upper bound 4 for the number of binary squares, a stronger result than obtained using the classical approach.

Our main lemma is

► Lemma 5.

- (a) Every length-n integer, n odd, $n \ge 13$, is the sum of binary squares as follows: either
 - one of length n-1 and one of length n-3, or
 - two of length n-1 and one of length n-3, or
 - one of length n-1 and two of length n-3, or
 - one each of lengths n-1, n-3, and n-5, or
 - two of length n-1 and two of length n-3, or
 - two of length n-1, one of length n-3, and one of length n-5.

- (b) Every length-n integer, n even, $n \ge 18$, is the sum of binary squares as follows: either
 - \blacksquare two of length n-2 and two of length n-4, or
 - three of length n-2 and one of length n-4, or
 - \bullet one each of lengths n, n-4, and n-6, or
 - two of length n-2, one of length n-4, and one of length n-6.

Lemma 5 almost immediately proves Theorem 1:

Proof. If $N < 2^{17} = 131072$, the result can be proved by a completely straightforward computation using dynamic programming: to form the sumset $S \oplus T$, given finite sets of natural numbers S and T, we use a bit vector corresponding to the elements of S, and then take its XOR shifted by each element of T. When we do this, we find that there are

- \sim 256 binary squares $< 2^{17}$;
- 19542 numbers $< 2^{17}$ that are the sum of two binary squares;
- = 95422 numbers $< 2^{17}$ that are the sum of three binary squares;
- 131016 numbers $< 2^{17}$ that are the sum of four binary squares.

Otherwise $N \ge 2^{17}$, so $(N)_2$ is a binary string of length $n \ge 18$. If n is odd, the result follows from Lemma 5 (a). If n is even, the result follows from Lemma 5 (b).

It now remains to prove Lemma 5. We do this in the next section.

4 Proof of Lemma 5

In this section we prove Lemma 5 in detail.

Proof. The basic idea is to use nondeterministic finite automata (NFAs). These are finite-state machines where each input corresponds to multiple computational paths; an input is accepted iff *some* computational path leads to a final state. We assume the reader is familiar with the basics of this theory; if not, please consult, e.g., [8]. For us, an NFA is a quintuple $(Q, \Sigma, \delta, q_0, F)$, where Q is the set of states, Σ is the input alphabet, δ is the transition function, q_0 is the initial state, and F is the set of final states.

We construct an NFA that, on input an integer N written in binary, "guesses" a representation as a sum of binary squares, and then verifies that the sum is indeed N. Everything is done using a reversed representation, with least significant digits processed first. There are some complications, however.

First, with an NFA we cannot verify that a guessed string is indeed a binary square, as the language $\{xx:x\in 1\{0,1\}^*\}$ is not a regular language. So instead we only guess the "first half" of a binary square. Now, however, we are forced to choose a slightly unusual representation for N, in order to be able to compare the sum of our guessed powers with the input N. If N were represented in its ordinary base-2 representation, this would be impossible with an NFA, since once we process the guessed "first half" and compare it to the input, we would no longer have the "second half" (identical to the first) to compare to the rest of the input.

To get around this problem, we represent integers N in a kind of "folded representation" over the input alphabet $\Sigma_2 \cup (\Sigma_2 \times \Sigma_2)$, where $\Sigma_k = \{0, 1, \dots, k-1\}$. The idea is to present our NFA with two bits of the input string at once, so that we can add both halves of our guessed powers at the same time, verifying that we are producing N as we go. Note that we use slightly different representations for the two parts of Lemma 5. The precise representations are detailed in their respective subsections.

We can now prove Lemma 5 by phrasing it as a language inclusion problem. For each of the two parts of the lemma, we can build an NFA A that only accepts such folded strings if

they repesent numbers that are the sum of any of the combination of squares as described in the lemma. We also create an NFA, B, that accepts all valid folded representations that are sufficiently long. We then check the assertion that the language recognized by B is a subset of that recognized by A.

4.1 Odd-length inputs

Again, to flag certain positions of the input tape, we use an extended alphabet. Define

$$\Gamma = \{1_f\} \ \cup \ \bigcup_{\alpha \in \{a,b,c,d,e\}} \{[0,0]_\alpha, [0,1]_\alpha, [1,0]_\alpha, [1,1]_\alpha\}.$$

Let N be an integer, and let n = 2i + 1 be the length of its binary representation. We write $(N)_2 = a_{2i}a_{2i-1}\cdots a_1a_0$ and fold this to produce the input string

$$[a_i, a_0]_a[a_{i+1}, a_1]_a \cdots [a_{2i-5}, a_{i-5}]_a[a_{2i-4}, a_{i-4}]_b[a_{2i-3}, a_{i-3}]_c[a_{2i-2}, a_{i-2}]_d[a_{2i-1}, a_{i-1}]_e a_{2i_f}.$$

Let $A_{\rm odd}$ be the NFA that recognizes those odd-length integers, represented in this folded format, that are the sum of binary squares meeting any of the 6 conditions listed in Lemma 5 (a). We construct $A_{\rm odd}$ as the union of several automata $A(t_{n-1},t_{n-3},m_a)$ and $B(t_{n-1},t_{n-3},t_{n-5},m_b)$. The parameters t_p represent the number of summands of length p we are guessing. The parameters m_a and m_b are the carries that we are guessing will be produced by the first half of the summed binary squares. A-type machines try summands of lengths n-1 and n-3 only, while B-type machines include at least one (n-5)-length summand. We note that for the purpose of summing, guessing t binary squares is equivalent to guessing a single square over the larger alphabet Σ_{t+1} .

We now consider the construction of a single automaton

$$A(t_{n-1}, t_{n-3}, m) = (Q \cup \{q_{\text{acc}}, q_0, s_1\}, \Gamma, \delta, q_0, \{q_{\text{acc}}\}).$$

The elements of Q have 4 non-negative parameters and are of the form $q(x_1, x_2, c_1, c_2)$. Because the t_{n-3} summand is not aligned with the input, we use our states to "remember" our guesses. When we make a guess at the higher end of the t_{n-3} summand, it must be used as the guess for its lower end on the *next step*. We remember this guess by storing it as the x_2 parameter. The parameter $x_1 \leq t_{n-3}$ is the last digit of the guessed summand of length n-3. We use c_1 to track the higher carry, and c_2 to track the lower carry. We must have $c_1, c_2 < t_{n-1} + t_{n-3}$.

We now discuss the transition function, δ of our NFA. In this section, we say that the sum of natural numbers, μ_1 and μ_2 , "produces" an output bit of $\theta \in \Sigma_2$ with a "carry" of γ if $\mu_1 + \mu_2 \equiv \theta \pmod{2}$ and $\gamma = \lfloor \frac{\mu_1 + \mu_2}{2} \rfloor$.

We allow a transition from q_0 to $q(x_1, x_2, c_1, c_2)$ on the letter $[j, k]_a$ iff there exists $0 \le r \le t_{n-1}$ such that $x_2 + r + m$ produces an output of j with a carry of c_1 and $x_1 + r$ produces an output of k with a carry of c_2 .

We allow a transition from $q(x_1, x_2, c_1, c_2)$ to $q(x'_1, x'_2, c'_1, c'_2)$ on the letters $[j, k]_a$ and $[j, k]_b$ iff there exists $0 \le r \le t_{n-1}$ such that $x'_2 + r + c_1$ produces an output of j with a carry of c'_1 and $x_2 + r + c_2$ produces an output of k with a carry of c'_2 . Elements of Q have identical transitions on inputs with subscripts a and b. The reason we have the letters with subscript b is for B-machines, which guess a summand of length n-5.

There is only one letter of the input with the subscript c, and it corresponds to the last higher guess of the summand of length n-3. We allow a transition from $q(x_1, x_2, c_1, c_2)$ to $q(x'_1, t_{n-3}, c'_1, c'_2)$ on the letter $[j, k]_c$ iff there exists $0 \le r \le t_{n-1}$ such that $t_{n-3} + r + c_1$

produces an output of j with a carry of c'_1 and $x_2 + r + c_2$ produces an output of k with a carry of c'_2 .

There is only one letter of the input with the subscript d, and it corresponds to the secondlast lower guess of the summand of length n-3. We allow a transition from $q(x_1, t_{n-3}, c_1, c_2)$ to $q(x'_1, 0, c'_1, c'_2)$ on the letter $[j, k]_d$ iff there exists $0 \le r \le t_{n-1}$ such that $r + c_1$ produces an output of j with a carry of c'_1 and $t_{n-3} + r + c_2$ produces an output of k with a carry of c'_2 .

There is only one letter of the input with the subscript e, and it corresponds to the last lower guess of the summand of length n-3. We allow a transition from $q(x_1, 0, c_1, c_2)$ to s_1 on the letter $[j, k]_e$ iff $t_{n-1} + c_1$ produces an output of j with a carry of 1 and $x_1 + t_{n-1} + c_2$ produces an output of k with a carry of k.

Finally, we add a transition from s_1 to q_{acc} on the letter 1_f .

We now consider the construction of a single automaton

$$B(t_{n-1}, t_{n-3}, t_{n-5}, m) = (P \cup Q \cup \{q_{\text{acc}}, q_0, s_1\}, \Gamma, \delta, q_0, \{q_{\text{acc}}\}).$$

The elements of P have 6 non-negative parameters and are of the form $q(x_1, x_2, y_1, y_3, c_1, c_2)$. The parameter $x_1 \leq t_{n-3}$ is the last digit of the guessed summand of length n-3 and $x_2 \leq t_{n-3}$ is the previous higher guess of the length-n-3 summand. The parameter $y_1 \leq t_{n-5}$ is the last digit of the guessed summand of length n-5 and $y_3 \leq t_{n-5}$ is the previous higher guess of the length-n-5 summand. We use c_1 to track the higher carry, and c_2 to track the lower carry. We must have $c_1, c_2 < t_{n-1} + t_{n-3} + t_{n-5}$. The elements of Q have 8 non-negative parameters and are of the form

$$q(x_1, x_2, y_1, y_2, y_3, y_4, c_1, c_2).$$

The parameter $x_1 \leq t_{n-3}$ is the last digit of the guessed summand of length n-3 and $x_2 \leq t_{n-3}$ is the previous higher guess of the length-n-3 summand. The parameters $y_1, y_2 \leq t_{n-5}$ are the last digit and the second-last digit of the guessed summand of length n-5 respectively. The parameter $y_3, y_4 \leq t_{n-5}$ are the two most recent higher guess of the length-n-5 summand, with y_4 being the most recent one. We use c_1 to track the higher carry, and c_2 to track the lower carry. We must have $c_1, c_2 < t_{n-1} + t_{n-3} + t_{n-5}$.

We now discuss the transition function, δ of our NFA. We allow a transition from q_0 to $p(x_1, x_2, y_1, y_3, c_1, c_2)$ on the letter $[j, k]_a$ iff there exists $0 \le r \le t_{n-1}$ such that $x_2 + y_3 + r + m$ produces an output of j with a carry of c_1 and $x_1 + y_1 + r$ produces an output of k with a carry of c_2 .

We use a transition from $p(x_1, x_2, y_1, y_3, c_1, c_2)$ to $q(x_1, x_2', y_1, y_2', y_3, y_4', c_1', c_2')$ on the letter $[j, k]_a$ iff there exists $0 \le r \le t_{n-1}$ such that $x_2' + y_4' + r + c_1$ produces an output of j with a carry of c_1 and $x_2 + y_2' + r + c_2$ produces an output of k with a carry of c_2 .

We use a transition from $q(x_1, x_2, y_1, y_2, y_3, y_4, c_1, c_2)$ to $q(x_1, x_2', y_1, y_2, y_4, y_4', c_1', c_2')$ on the letter $[j, k]_a$ iff there exists $0 \le r \le t_{n-1}$ such that $x_2' + y_4' + r + c_1$ produces an output of j with a carry of c_1 and $c_2' + c_2' + c_3' + c_4' + c_5' +$

We use a transition from $q(x_1, x_2, y_1, y_2, y_3, t_{n-5}, c_1, c_2)$ to $q(x_1, x_2', y_1, y_2, t_{n-5}, t_{n-5}, c_1', c_2')$ on the letter $[j, k]_b$ iff there exists $0 \le r \le t_{n-1}$ such that $x_2' + r + c_1$ produces an output of j with a carry of c_1 and $x_2 + y_3 + r + c_2$ produces an output of k with a carry of k.

We use a transition from $q(x_1, x_2, y_1, y_2, t_{n-5}, t_{n-5}, c_1, c_2)$ to $q(x_1, t_{n-3}, y_1, y_2, t_{n-5}, t_{n-5}, c'_1, c'_2)$ on the letter $[j, k]_c$ iff there exists $0 \le r \le t_{n-1}$ such that $t_{n-3} + r + c_1$ produces an output of j with a carry of c_1 and $x_2 + y_3 + r + c_2$ produces an output of k with a carry of k

We use a transition from $q(x_1, t_{n-3}, y_1, y_2, t_{n-5}, t_{n-5}, c_1, c_2)$ to $q(x_1, t_{n-3}, y_1, y_2, t_{n-5}, t_{n-5}, c'_1, c'_2)$ on the letter $[j, k]_d$ iff there exists $0 \le r \le t_{n-1}$ such that $r + c_1$ produces an

output of j with a carry of c_1 and $t_{n-3} + y_1 + r + c_2$ produces an output of k with a carry of c_2 .

We use a transition from $q(x_1, t_{n-3}, y_1, y_2, t_{n-5}, t_{n-5}, c_1, c_2)$ to s_1 on the letter $[j, k]_e$ iff $t_{n-1} + c_1$ produces an output of j with a carry of 1 and $x_1 + y_2 + t_{n-1} + c_2$ produces an output of k with a carry of k.

Finally, we add a transition from s_1 to q_{acc} on the letter 1_f .

We now turn to verification of the inclusion assertion. We used the Automata Library toolchain of the ULTIMATE program analysis framework [7, 6] to establish our results. The ULTIMATE code proving our result can be found in the file OddSquareConjecture.ats at https://cs.uwaterloo.ca/~shallit/papers.html. Since the constructed machines get very large, we wrote a C++ program generating these machines, which can be found in the file OddSquares.cpp at the same location.

The final machine, A_{odd} , has 2258 states. The syntax checker, B, has 8 states. We then asserted that the language recognized by B is a subset of that recognized by A. ULTIMATE verified this assertion in under a minute. Since this test succeeded, the proof of Lemma 5 (a) is complete.

4.2 Even-length inputs

In order to flag certain positions of the input tape, we use an extended alphabet. Define

$$\Gamma = \left(\bigcup_{\alpha \in \{a,b,c,d,e\}} \{ [0,0]_{\alpha}, [0,1]_{\alpha}, [1,0]_{\alpha}, [1,1]_{\alpha} \} \right) \cup \left(\bigcup_{\beta \in \{f,g,h,i\}} \{0_{\beta},1_{\beta}\} \right).$$

Let N be an integer, and let n=2i+4 be the length of its binary representation. We write $(N)_2=a_{2i+3}a_{2i+2}\cdots a_1a_0$ and fold this to produce the input string

$$[a_{i}, a_{0}]_{a}[a_{i+1}, a_{1}]_{b}[a_{i+2}, a_{2}]_{c}[a_{i+3}, a_{3}]_{c} \cdots \\ \cdots [a_{2i-3}, a_{i-3}]_{c}[a_{2i-2}, a_{i-2}]_{d}[a_{2i-1}, a_{i-1}]_{e}a_{2i_{1}}a_{2i+1_{a}}a_{2i+2_{b}}a_{2i+3_{i}}.$$

Let A_{even} be the NFA that recognizes the even-length integers, represented in this folded format, iff the integer is the sum of binary squares meeting any of the 4 conditions listed in Lemma 5 (b). We construct A_{even} as the union of several automata $A(t_n, t_{n-2}, t_{n-4}, t_{n-6}, m)$. The parameters t_p represent the number of summands of length p we are guessing. The parameter m is the carry that we are guessing will be produced by the first half of the summed binary squares. Again, guessing t binary squares is equivalent to guessing a *single* square over the larger alphabet Σ_{t+1} .

We now consider the construction of a single automaton

$$A(t_n, t_{n-2}, t_{n-4}, t_{n-6}, m) = (Q \cup \{q_{\rm acc}\}, \Gamma, \delta, q_0, \{q_{\rm acc}\}).$$

The elements of Q have 8 non-negative parameters and are of the form $q(x_1, x_2, x_3, y_1, z_1, z_2, c_1, c_2)$. The parameter x_1 is the second digit of the guessed summand of length n. The parameters x_2 and x_3 represent the previous 2 lower guesses of the length-n summand; these must be the next 2 higher guesses of this summand. The parameter y_1 represents the previous lower guess of the length-(n-2) summand. We set z_1 as the last digit of the guessed summand of length n-6, while z_2 is the previous higher guess of this summand. Finally, c_1 tracks the lower carry, while c_2 tracks the higher carry. For any p, we must have $x_p \leq t_n, y_p \leq t_{n-2}, z_p \leq t_{n-6}$, and $c_p < t_n + t_{n-2} + t_{n-4} + t_{n-6}$. The initial state, q_0 , is q(0,0,0,0,0,0,0).

We now discuss the transition function, δ of our NFA. Note that in our representation of even-length integers, the first letter of the input must have the subscript a, and it is the only letter to do so. We only allow the initial state to have outgoing transitions on such letters.

We allow a transition from q_0 to $q(x_1, 0, x_3, y_1, z_1, z_2, c_1, c_2)$ on the letter $[j, k]_a$ iff there exists $0 \le r \le t_{n-4}$ such that $x_1 + t_{n-2} + r + z_2 + m$ produces an output of j with a carry of c_2 and $x_3 + y_1 + r + z_1$ produces an output of k with a carry of k.

The second letter of the input must have the subscript b, and it is the only letter to do so. We allow a transition from $q(x_1,0,x_3,y_1,z_1,z_2,c_1,c_2)$ to $q(x_1,x_3,x_3',y_1',z_1,z_2',c_1',c_2')$ on the letter $[j,k]_b$ iff there exists $0 \le r \le t_{n-4}$ such that $t_n+y_1+r+z_2'+c_2$ produces an output of j with a carry of c_2' and $x_3'+y_1'+r+z_2+c_1$ produces an output of k with a carry of c_1' .

We allow a transition from $q(x_1, x_2, x_3, y_1, z_1, z_2, c_1, c_2)$ to $q(x_1, x_3, x_3', y_1', z_1, z_2', c_1', c_2')$ on the letter $[j, k]_c$ iff there exists $0 \le r \le t_{n-4}$ such that $x_2 + y_1 + r + z_2' + c_2$ produces an output of j with a carry of c_2' and $x_3' + y_1' + r + z_2 + c_1$ produces an output of k with a carry of c_1' .

The letter of the input with the subscript d corresponds to the last guess of the lower half of the summand of length n-6, and it is the only letter to do so. We allow a transition from $q(x_1, x_2, x_3, y_1, z_1, t_{n-6}, c_1, c_2)$ to $q(x_1, x_3, x_3', y_1', z_1, 0, c_1', c_2')$ on the letter $[j, k]_d$ iff there exists $0 \le r \le t_{n-4}$ such that $x_2 + y_1 + r + c_2$ produces an output of j with a carry of c_2' and $x_3' + y_1' + r + t_{n-6} + c_1$ produces an output of k with a carry of c_1' .

The letter of the input with the subscript e corresponds to the last guess of both halves of the summand of length n-4, and it is the only letter to do so. We allow a transition from $q(x_1,x_2,x_3,y_1,z_1,0,c_1,c_2)$ to $q(x_1,x_3,x_3',y_1',0,0,0,c_2')$ on the letter $[j,k]_e$ iff $x_2+y_1+t_{n-4}+c_2$ produces an output of j with a carry of c_2' and $x_3'+y_1'+t_{n-4}+z_1+c_1$ produces an output of k with a carry of k.

We allow a transition from $q(x_1, x_2, x_3, y_1, 0, 0, 0, c_2)$ to $q(x_1, x_3, 0, 0, 0, 0, c_2)$ on the letter j_f iff $x_2 + y_1 + c_2$ produces an output of j with a carry of c_2 .

We allow a transition from $q(x_1, x_2, 0, 0, 0, 0, c_2)$ to $q(x_1, 0, 0, 0, 0, 0, c_2)$ on the letter j_g iff $x_2 + t_{n-2} + c_2$ produces an output of j with a carry of c_2 .

We allow a transition from $q(x_1, 0, 0, 0, 0, 0, c_2)$ to $q(0, 0, 0, 0, 0, 0, c_2)$ on the letter j_h iff $x_1 + c_2$ produces an output of j with a carry of c_2 .

We allow a transition from $q(0, 0, 0, 0, 0, 0, 0, c_2)$ to q_{acc} on the letter 1_i iff $t_n + c_2$ produces an output of 1 with a carry of 0.

The final machine, $A_{\rm even}$ is constructed as the union of 15 automata:

- A(0,2,2,0,m), varying m from 0 to 3
- \blacksquare A(0,3,1,0,m), varying m from 0 to 3
- A(1,0,1,1,m), varying m from 0 to 2
- \blacksquare A(0,2,1,1,m), varying m from 0 to 3

We now turn to verification of the inclusion assertion. The ULTIMATE code proving our result can be found in the file EvenSquareConjecture.ats at https://cs.uwaterloo.ca/~shallit/papers.html. Since the constructed machines get very large, we wrote a C++ program generating these machines, which can be found in the file EvenSquares.cpp at the same location.

The final machine, $A_{\rm even}$, has 1343 states. The syntax checker, B, has 12 states. We then asserted that the language recognized by B is a subset of that recognized by A. ULTIMATE verified this assertion in under a minute. Since this test succeeded, the proof of Lemma 5 (b) is complete.

▶ Corollary 6. Given an integer N > 686, we can find an expression for N as the sum of four binary squares in time linear in $\log N$.

Proof. For N < 131072, we do this with a simple brute-force search via dynamic programming, as explained previously. Otherwise we construct the appropriate automaton A (depending on whether the binary representation of N has either even or odd length). Now carry out the usual direct product construction for intersection of languages on A and B, where B is the automaton accepting the folded binary representation of N. The resulting automaton has at most $c \log N$ states and transitions. Now use the usual depth-first search of the transition graph to find a path from the initial state to a final state. The labels of this path gives the desired representation.

4.3 Ensuring correctness

As in every machine-based proof, we want some assurance that our calculations were correct. We tested our machine by calculating those integers of length 8 that can be expressed as the sum of up to 3 binary squares of length 4, and up to 4 binary squares of length 6. We then used the ULTIMATE framework to test that those length-8 integers are accepted

by our machine, but all others are rejected. The code running this test can be found as Minus2Minus4SquareConjecture - Test 1 at https://cs.uwaterloo.ca/ shallit/papers.html.

We also tested the machine by calculating those integers of length 10 that can be expressed as the sum of up to to 2 binary squares of length 6, and up to 4 binary squares of length 8. We then built the analogous machine and confirmed that these length-10 integers are accepted, but all others are rejected. We then repeated this test for those integers of length 10 that can be expressed as the sum of up to to 3 binary squares of length 6, and up to 3 binary squares of length 8. The code running these tests can be found as Minus2Minus4SquareConjecture - Test 2 and Minus2Minus4SquareConjecture - Test 3 at https://cs.uwaterloo.ca/~shallit/papers.html.

5 Optimality

In this section we show that the "4" in Theorem 1 is optimal.

▶ **Theorem 7.** For $n \ge 1$, n odd, $n \ne 9$, the number 2^n is not the sum of three or fewer (positive) binary squares.

Proof. Let $m \ge 0$ and n = 2m + 1 be odd. The cases m = 0, 1, 2, 3 are easy to verify by hand, so assume $m \ge 4$.

In what follows we distinguish between "mod" used in the ordinary notion of congruence (where $x \equiv a \pmod{b}$ means that b divides x - a), and the use of "mod" as a function, where $x = a \pmod{b}$ means both that $x \equiv a \pmod{b}$ and that $0 \le a < b$.

Clearly $N := 2^n$ is not a binary square.

Suppose N is the sum of two positive binary squares. The largest binary square < N is clearly $2^{2m} - 1$. Hence the sum of two binary squares is either larger than N, or no larger than $2(2^{2m} - 1) = 2^{2m+1} - 2 < N$, a contradiction.

The remaining case is that 2^{2m+1} is the sum of three binary squares, say N=A+B+C with

$$A = a(2^e + 1) > B = b(2^f + 1) > C = c(2^g + 1)$$

with $e \ge f \ge g$ and $2^{e-1} \le a < 2^e$, $2^{f-1} \le b < 2^f$, and $2^{g-1} \le c < 2^g$. Clearly $1 \le e, f, g \le m$.

We first observe that e=m. For otherwise, $e \leq m-1$ and the inequality $e \geq f \geq g$ implies

$$N = A + B + C \le 3(2^{m-1} - 1)2^{m-1} < 3 \cdot 2^{2m-2} < N$$

a contradiction.

Similarly, we observe that f = m. For otherwise

$$N = A + B + C < (2^{m} - 1)2^{m} + 2(2^{m-1} - 1)2^{m-1} < 3 \cdot 2^{2m-1} < N,$$

a contradiction.

Thus, setting d = a + b, we see that $N = d(2^m + 1) + c(2^g + 1)$ where $2^m \le d \le 2^{m+1} - 2$. Suppose $d = 2^{m+1} - 2$. Then $N = d(2^m + 1) + c(2^g + 1)$ implies that $C = c(2^g + 1) = 2$. But C = 2 is not a binary square. So in fact $2^m \le d \le 2^{m+1} - 3$.

Next we argue that g > m/2. For otherwise $g \le m/2$ and we have

$$N = d(2^{m}+1) + c(2^{g}+1) \le (2^{m+1}-3)(2^{m}+1) + (2^{m/2}-1)(2^{m/2}+1) = 2^{2m+1}-4 = N-4,$$

a contradiction.

Next we argue that g < m. For otherwise g = m and then $N = 2^{2m+1} = A + B + C = (a+b+c)(2^m+1)$. But then 2^{2m+1} is divisible by the odd number 2^m+1 , a contradiction.

Now consider the equation $N = d(2^m + 1) + c(2^g + 1)$ and take it modulo $2^m + 1$. We have $2^{2m+1} - 2 = 2(2^m - 1)(2^m + 1) \equiv 0 \pmod{2^m + 1}$, and so $N = 2^{2m+1} \equiv 2 \pmod{2^m + 1}$.

Thus we get

$$c(2^g + 1) \equiv 2 \pmod{2^m + 1}.$$
 (2)

It suffices to show that the congruence (2) has no solutions in the possible range for c, except when m = 4 and q = 3. In order to see this, we need a technical lemma.

▶ Lemma 8. Suppose $m, g \ge 1$ are integers with m/2 < g < m. Suppose c is an integer with $2^{g-1} \le c < 2^g$. Using Euclidean division, find the unique expression of c as $t \cdot 2^{m-g} + u$ for $0 \le u < 2^{m-g}$. Then

$$c(2^g + 1) \mod (2^m + 1) = t(2^{m-g} - 1) + u(2^g + 1).$$

Proof. We have

$$\begin{split} c(2^g+1) &= (t \cdot 2^{m-g} + u)(2^g+1) \\ &= t \cdot 2^m + t \cdot 2^{m-g} + u(2^g+1) \\ &= t(2^m+1) + t(2^{m-g}-1) + u(2^g+1) \\ &\equiv t(2^{m-g}-1) + u(2^g+1) \pmod{2^m+1}. \end{split}$$

This last congruence alone does not prove what we want; we also have to show that

$$0 \le t(2^{m-g} - 1) + u(2^g + 1) \le 2^m + 1$$

so that the residues don't "wrap around" when computed modulo $2^m + 1$. However, $t = |c/2^{m-g}| = 2^{2g-m} - 1$, and so

$$t(2^{m-g}-1) + u(2^g+1) \le (2^{2g-m}-1)(2^{m-g}-1) + (2^{m-g}-1)(2^g+1)$$
$$= 2^m - 2^{2g-m} < 2^m + 1.$$

as desired.

Now from the Lemma we see that the expression $c(2^g + 1) \mod (2^m + 1)$ achieves its smallest value when $c = 2^{g-1}$ (for then $t = 2^{2g-m-1}$ and u = 0), and this smallest value is $2^{2g-m-1}(2^{m-g}-1) > 2$, except when m = 4, g = 3.

▶ Remark. When m=4 and g=3, letting c=28 and d=4 we get the solution $512=2^9=28\cdot(2^4+1)+4\cdot(2^3+1)$. This corresponds to two distinct expressions of 2^9 as the sum of three binary squares: 512=255+221+36 and 512=238+238+36.

6 Other results

Our technique can be used to obtain other results in additive number theory. For example, recently Crocker [3] and Platt & Trudgian [14] studied the integers representable as the sum of two ordinary squares and two powers of 2. The analogue of this theorem is the following:

▶ Lemma 9.

- (a) Every length-n integer, n odd, $n \ge 7$, is the sum of at most two powers of 2 and either:
 - \blacksquare at most two binary squares of length n-1, or
 - \blacksquare at most one binary square of length n-1 and one of length n-3.
- (b) Every length-n integer, n even, $n \ge 10$, is the sum of at most two powers of 2 and either:
 - \blacksquare at most one binary square of length n and one of length n-4, or
 - at most one binary square of length n-2 and one of length n-4.

Proof. We use a similar proof strategy as before. The ULTIMATE code proving our result can be found in the files OddSquarePowerConjecture.ats and EvenSquarePowerConjecture.ats at https://cs.uwaterloo.ca/~shallit/papers.html; there one can also find the generators can be found as OddSquarePower.cpp and EvenSquarePower.cpp.

The final machines for the odd-length and even-length cases have 806 and 2175 states respectively. The language inclusion assertions all hold. This concludes the proof.

We thus have the following theorem:

▶ **Theorem 10.** Every natural number N is the sum of at most two binary squares and at most two powers of 2.

Proof. For N < 512, the result can be easily verified. Otherwise, we use Lemma 9 (a) if N is an odd-length binary number and Lemma 9 (b) if it is even.

We also consider the notion of generalized binary squares. A number N is called a generalized binary square if one can concatenate 0 or more leading zeroes to its binary representation to produce a binary square. As an example, 9 is a generalized binary square, since 9 in base 2 is 1001, which can be written as 001001 = (001)(001). The first few generalized binary squares are

```
0, 3, 5, 9, 10, 15, 17, 18, 27, 33, 34, 36, 45, 51, 54, 63, \ldots;
```

they form sequence $\underline{A175468}$ in the OEIS [18].

In what follows, when we refer to the length of a generalized binary square, we mean the length including the leading zeroes. Thus, 9 is a generalized binary square of length 6 (and not 4).

▶ Lemma 11.

(a) Every length-n integer, $n \ge 7$, n odd, is the sum of 3 generalized binary squares, of lengths n+1, n-1, and n-3.

(b) Every length-n integer, $n \geq 8$, n even, is the sum of 3 generalized binary squares, of lengths n, n-2, and n-4.

Proof. We use a very similar proof strategy as in the proof of Lemma 5. We drop the requirement that the most significant digit of our guessed squares be 1, thus allowing for generalized binary squares. Note that the square of length n + 1 in part (a) must start with a 0.

The ULTIMATE code proving our result can be found in the files OddGenSquareConjecture. ats and EvenGenSquareConjecture.ats at https://cs.uwaterloo.ca/~shallit/papers.html; there one can also find the generators OddGeneralizedSquares.cpp and EvenGeneralizedSquares.cpp. The final machines for the odd-length and even-length cases have 132 and 263 states respectively.

We thus have the following theorem:

▶ Theorem 12. Every natural number N > 7 is the sum of 3 generalized binary squares.

Proof. For 7 < N < 64 the result can be easily verified. Otherwise, we use Lemma b (a) is an odd-length binary number and Lemma b (b) if it is even.

7 Further work

Numerical evidence suggests the following two conjectures:

▶ Conjecture 13. Let α_3 denote the lower asymptotic density of the set S_3 of natural numbers that are the sum of three binary squares. Then $\alpha_3 < 0.9$.

We could also focus on sums of *positive* binary squares. (For the analogous problem dealing with ordinary squares, see, e.g., [5, Chapter 6].) It seems likely that our method could be used to prove the following result.

▶ Conjecture 14. Every natural number > 1772 is the sum of exactly four positive binary squares. There are 112 exceptions, given below:

```
0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 13, 14, 15, 16, 17, 18, 20, 21, 22, 23, 25, 27, 28, 29, 30, 32, 34, 35, 37, 39, 41, 42, 44, 46, 47, 49, 51, 53, 56, 58, 62, 65, 67, 74, 83, 88, 95, 100, 104, 107, 109, 113, 116, 122, 125, 131, 134, 140, 143, 148, 149, 155, 158, 160, 161, 167, 170, 173, 175, 182, 184, 368, 385, 402, 407, 419, 424, 436, 441, 458, 475, 492, 509, 526, 543, 552, 560, 569, 587, 599, 608, 613, 620, 625, 638, 647, 653, 671, 686, 698, 713, 1508, 1541, 1574, 1607, 1640, 1673, 1706, 1739, 1772.
```

Other interesting things to investigate include estimating the number of distinct representations of N as a sum of four binary squares, both in the case where order matters, and where order does not matter. These are sequences A290335 and A298731 in the OEIS, respectively.

In recent work [9] it was proved, using a combinatorial and number-theoretic approach, that the binary k'th powers form an asymptotic basis of finite order for the multiples of $gcd(k, 2^k - 1)$. However, the constant obtained thereby is rather large.

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