A binomial representation of the 3x + 1 problem

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Abstract

We show how the 3x + 1 conjecture can be expressed in the language of arithmetical formulas with binomial coefficients.

1 Introduction

1.1 The 3x + 1 problem

The 3x+1 problem is known under different names. It is also often called Collatz's problem, Ulam's problem, Syracuse problem and by some other names. The problem can be stated as follows.

Consider the following simple transformation of positive integers:

$$f(x) = \begin{cases} \frac{3x+1}{2}, & \text{if } x \text{ is odd}; \\ \frac{x}{2}, & \text{if } x \text{ is even.} \end{cases}$$
(1)

Consider further its iteration g defined recursively as

$$g(a,0) = a g(a,k+1) = f(g(a,k)),$$
(2)

i.e. $g(a,k) = f(f(\dots f(a)\dots))$ where f is applied k times. At last, define a relation Syr between positive integers a and b by:

$$\operatorname{Syr}(a,b) \iff \exists m \ g(a,m) = b.$$
 (3)

We say that a number m such that g(a, m) = b realizes Syr(a, b) which clearly means that m successive applications of f transform a into b.

It can be verified, by hand for very small values of a and by computer for relatively small values of a, that Syr(a, 1) holds and hence the sequence of

iterated values $a, f(a), f(f(a)), \ldots$ eventually becomes periodic ..., 1, 2, 1, 2, 1, 2, ... The problem is to prove that this is in fact true for all a.

The literature devoted to this deceptively simply stated problem is very vast; the reader can consult [6] for an introduction to this field and [7], [8] and [19] for the recent state of the art. It should be noticed that the simulation of this computation by very small computing systems has been devised: see, for instance, [14] and, more recent paper, [10].

1.2 The language of binomial expressions

In the first half of XX century the process of formalization of mathematics reached some culminating point thanks to Gödel who showed that many mathematical statements can be expressed by arithmetical formulas, i.e. by formulas of the form

$$\mathbf{Q}_1 x_1 \mathbf{Q}_2 x_2 \ldots \mathbf{Q}_k x_k G(x_1, x_2, \ldots, x_k)$$

$$\tag{4}$$

where the Q's are universal or existential quantifiers, variables x_1, \ldots, x_k range over the set of natural numbers, and G is a quantifier-free formula constructed, according to conventional rules, from x_1, \ldots, x_k and particular natural numbers by arithmetical operations of addition, subtraction and multiplication, relation of equality and logical operations AND, OR and NOT.

About forty years later, Davis-Matiyasevich-Putnam-Robinson established the negative answer to the Tenth Hilbert's problem, by proving that if all universal quantifier in (4) are bounded (which is often the case) then they can be replaced by extra existential quantifiers which together with other simplifications leads to purely existential formulas of the form

$$\exists x_1 \exists x_2 \dots \exists x_m P(x_1, \dots, x_m) = 0$$
(5)

where $x_1 \ldots, x_m$ range over the set of natural numbers and $P(x_1, \ldots, x_m)$ is a polynomial with integer coefficients (see, for example, [1] or [13] where the Goldbach's conjecture and the Riemann Hypothesis are expressed as the undecidability of particular Diophantine equations).

It is interesting to note that the binomial coefficients played the key role on the intermediate steps in transformation of (4) into (5) starting from pioneer work [2] and finishing with modern techniques presented in [13]. But what could be the reason to allow binomial coefficients in final arithmetical formulas now that we know thanks to (5) that the binomial coefficients can be eventually eliminated?

At least two different answers to this question can be given.

First, an arithmetical formula with binomial coefficients can be much shorter than an equivalent to it arithmetical formula containing only operations of addition, subtraction and multiplication.

Second, when congruence with fixed modulo is used as the predicate symbol instead of the equality relation (as it is done in Theorem 1 below), the existential quantifiers can, under some conditions, be replaced by summation (as in

 $\mathbf{2}$

Corollary 1 below). In its turn, recently we witness a spectacular progress in computer search of closed forms for sums of products of binomial coefficients (see [15, 18] for accounts on this approach and for example of non-trivial results obtained this way). This use of computers has the following nice feature: even if it took several CPU hours to find a closed form, the verification of the found identity can be acceptible for a human-being, which opens new ways to atacking old problems.

That is why it is so interesting to translate mathematical problems, when possible, to the language of binomial coefficients. This language turned out to have surprisinly great expressive power. For example, recently the second author [12] (see also [17]) was able to restate in this way the famous Four Colour Conjecture. In [4] Fermat's last theorem was translated into the language of binomial expressions. An earlier examples are Mann-Shanks [9] criterion of primality in terms of divisibility of several binomial coefficients and second author criteria [11] of primality, twin primality, Mersenne and Fermat numbers primality expressed in terms of divisibility or non-divisibility of a single binomial coefficient at the expense of usage of exponentiation and division.

In section 2.4 we present 3 restatements of the 3x + 1 problem by arithmetical formulas with binomial coefficients.

2 Modelling the 3x + 1 problem

2.1 Prelimiary tools

Let a, b be natural numbers (by which we understand non-negative integers). Their binary representation will respectively be written as $\sum_{i=0}^{m} \alpha_i 2^i$ with $\alpha_i \in \{0,1\}$, and $\sum_{i=0}^{m} \beta_i 2^i$ with $\beta_i \in \{0,1\}$. It is clear that by padding initial zeros, it may be assumed that the above summations run over the same range for both a and b.

Define now the following relation between a and b:

$$a \preceq b \quad \Longleftrightarrow \quad \forall i \; \alpha_i \leq \beta_i,$$
 (6)

which is independent of the value of m used for the binary representation of both a and b. Relation $a \leq b$ is read: "b masks a" or "a is masked by b".

As an example, take:

here $a \leq c, b \leq c$ but $a \not\leq b$.

It turned out that the masking relation can be easily expressed via binomial coefficients:

LEMMA 1. For any natural numbers a and b we have:

$$a \preceq b \iff \begin{pmatrix} b \\ a \end{pmatrix} \equiv 1 \pmod{2}.$$
 (7)

PROOF. The lemma follows immediately from a theorem due to Kummer [5] (for modern presentation see, for example, [16]). For the sake of completeness, a proof of Kummer's theorem is given as an appendix to this paper. \blacksquare

Another relation, very useful in the sequel, is defined as follows:

$$a \perp b \iff \forall i \; \alpha_i \beta_i = 0 \iff \sum_i \alpha_i \beta_i = 0.$$
 (8)

The relation of orthogonality $a \perp b$ can be expressed by means of the masking relation (and hence by binomial coefficients as well) as it is stated by the following result:

LEMMA 2. For any natural numbers a and b, $a \perp b$ if and only if $a \preceq a + b$. PROOF. Consider the occurrence of the first carry, if any, when adding a and b.

In its turn, it is easy to express by means of \bot the property "to be a power of 2":

LEMMA 3. For any positive number v, there is a number k such that $v = 2^k$ if and only if $v \perp v - 1$.

In order to avoid subtractions in formulas, we shall work with numbers which are powers of 2 minus 1.

LEMMA 4. Let $w + 1 = 2^k$ for some k. A natural number u is of the form $\sum_{i=0}^m (4w+4)^i$ for some m if and only if $u \leq (4w+4)u+1$. PROOF. The binary notation of a number u of the required form looks like

$$1 \underbrace{0 \dots 0}_{k+1} 1 \underbrace{0 \dots 0}_{k+1} 1 \dots 1 \underbrace{0 \dots 0}_{k+1} 1 \tag{9}$$

and is completely characterized by the following properties:

- the binary digits of u in positions $2^1, 2^2, \ldots, 2^{k+1}$ are equal to 0;
- every (i + k + 2)nd digit is less or equal to the *i*th digit.

Multiplication by 4w + 4 corresponds to shifting to k + 2 digits so number (4w + 4)u + 1 itself has zeros in positions $2^1, 2^2, \ldots, 2^{k+1}$ and thus condition $u \leq (4w + 4)u + 1$ is equivalent to the two above stated characteristic properties.

2.2 Representations of finite sequences

Consider a finite sequence of natural numbers

$$X = \langle x_1, \dots, x_m \rangle. \tag{10}$$

Let $w + 1 = 2^k$ be a power of 2 so big that

$$x_i < 4w + 4, \quad i = 1, \dots, m.$$
 (11)

We shall say that the number

$$Q = \sum_{i=1}^{m} x_i (4w+4)^{i-1}$$
(12)

w-represents the sequence (10) or is a *w*-representation of the sequence (10). Thanks to condition (11), the binary notation of Q is constituted by the binary notations of x_1, \ldots, x_m padded, if necessary, by leading zeros to the length k+2.

Here is an example: the binary notation of the number which 63-represents sequence (18, 9, 14, 7) is

$$\underbrace{\underbrace{0000111}_{7}\underbrace{0001110}_{14}\underbrace{0001001}_{9}\underbrace{0010010}_{18}}_{18}$$
(13)

We see that three numbers, Q, w, and m, uniquely determine the original sequence (10). Namely, in order to restore the sequence, it is sufficient to cut the binary notation of Q into m blocks of length k + 2.

We shall say that number (12) strongly w-represents the sequence (10) or is a strong w-representation of the sequence (10) if condition (which is stronger than (11))

$$x_i < 2w + 2, \quad i = 1, \dots, m$$
 (14)

is satisfied.

We could express via binomial coefficients the relation "Q is a strong wrepresentation of a sequence". However, having in mind our final goal, the 3x+1problem, we proceed to another represention of sequences.

Define four functions π, ρ, σ, τ on natural numbers in the following way: if x = 2z + y with $y \in \{0, 1\}$, then

$$egin{aligned} \pi(x) &= (1-y), &
ho_{(}x) &= y, \ \sigma(x) &= (1-y)z, & au(x) &= yz \end{aligned}$$

Functions π and ρ determing the parity of their arguments, and the values of $\sigma(x)$ and $\tau(x)$ are equal either to $\lfloor x/2 \rfloor$ or to 0 depending of the parity of x. Respectively, for every x,

$$x = 2\sigma(x) + 2\tau(x) + \rho(x).$$
 (15)

Moreover, it is easy to check that, according to (1), the value of f(x) also can be expressed as a linear combination of the same numbers:

$$f(x) = \sigma(x) + 3\tau(x) + 2\rho(x).$$
 (16)

We shall use the following notation: if φ is a function from $I\!N$ into $I\!N$ then

$$\varphi(\langle x_1, \dots, x_m \rangle) = \langle \varphi(x_1), \dots, \varphi(x_m) \rangle.$$
(17)

Let Q be the number strongly w-representing some sequence (10). Let P, R, S, and T be the numbers representing the sequences $\pi(X), \rho(X), \sigma(X), \tau(X)$ respectively.

Continuing our example (13), we found the following binary representation:

Numbers P and R indicates the positions of even and odd elements in the sequence (10) respectively. Together with numbers S and T, this gives full information about the values of all elements in the sequence (10). We shall say that the four number P, R, S, and T form a *detailed w-representation* of the sequence (10).

According to (15), the number Q can be reconstructed as Q = 2S + 2T + R. What is important is the fact that from a detailed representation of sequence (10) we can also easily construct number F which is the *w*-representation of the sequence f(X). Namely, it follows from (16) that

$$F = S + 3T + 2R. (18)$$

Note that F need not be a strong representation, however, the condition (14) implies that $f(x_i) < 4w + 4$ what is required for the definition of a w-representation.

Let w + 1 be a power of 2. Suppose that we are given four numbers p, r, s, and t. We are now to state a condition which is necessary and sufficient for these numbers to form a detailed w-representation of some sequence (10).

First of all, numbers p and r should be orthogonal, i.e. they should satisfy condition

$$p \perp r.$$
 (19)

Second, the number p + r should be of the form (9), i.e., according to Lemma 4 it should satisfy the condition

$$p + r \leq (4w + 4)(p + r) + 1.$$
 (20)

Now it remains to impose conditions which whould restrict the positions at which the binary digits of s and t could be equal to 1, namely,

$$s \preceq wp, \qquad t \preceq wr$$
 (21)

(note that the binary notation of w looks like $1 \dots 1$).

Summing up, we get

LEMMA 5. Let w + 1 be a power of 2. Then four numbers p, r, s, and t form a detailed w-representation of some sequence if and only if they satisfy conditions (19), (20), and (21).

2.3 Representation of the Syr relation

Without loss of generality we can restrict ourself to even initial numbers, i.e., the 3x + 1 problem can be stated as $\forall a \operatorname{Syr}(2a, 1)$ and as $\forall a \operatorname{Syr}(2a, 2)$. Suppose now that some positive integer *m* realizes $\operatorname{Syr}(2a, b)$ for given *a* and *b*. This means that the equation

$$f(\langle 2a, x_1, \dots, x_{m-1} \rangle) = \langle x_1, \dots, x_{m-1}, b \rangle$$
(22)

has a solution

$$x_i = g(2a, i), \quad i = 1, \dots, m - 1.$$
 (23)

On the other hand, it is easy to see from the definitions (2) and (17) that every solution of equation (22) has the form (23) and, moreover, $f(x_{m-1}) = b$.

If w + 1 is a power of 2 so big that

$$2a < 2w + 2 \tag{24}$$

and numbers p, r, s, and t form the detailed *w*-representation of some sequence $\langle x_1, \ldots, x_{m-1} \rangle$ then it is easy to see that numbers

$$(4w+4)p+1,$$
 $(4w+4)r,$ $(4w+4)s+a,$ $(4w+4)t$

form the detailed representation of the sequence $\langle 2a, x_1, \ldots, x_{m-1} \rangle$ which is the argument of f in (22). Thus, according to (18), number

$$3((4w+4)t+a) + 2(4w+4)r + (4w+4)s$$

w-represents the sequence from the left-hand side in (22).

On the other hand, it is easy to check that if, in addition,

$$b \le w,$$
 (25)

then the sequence from the right-hand side of (22) is w-represented by the number $2(s+t) + r + (4w+4)^m b$. Thus we can rewrite the equation (22) as

$$2(s+t) + r + (4w+4)^m b = 3((4w+4)t + a) + 2(4w+4)r + (4w+4)s.$$
 (26)

According to Lemma 3, the condition that w + 1 is a power of 2 can be written as

$$w + 1 \perp w. \tag{27}$$

To eliminate the exponentiation which occurs in (26) it is sufficient to note that

$$(4w+4)^m = (4w+3)(p+r) + 1.$$
(28)

We can now sum up our argumentation as

LEMMA 6. Syr(2a, b) holds if and only if there are natural numbers w, p, r, s and t such that

$$a \leq w$$
 (29)

$$b \leq w$$
 (30)

$$w \perp w+1 \tag{31}$$

$$p \perp r$$
 (32)

$$p + r \leq 4(w+1)(p+r) + 1$$
 (33)

$$s \preceq pw$$
 (34)

$$t \preceq rw$$
 (35)

$$2s + 2t + r + b((4w + 3)(p + r) + 1) =$$

3((4w + 4)t + a) + 2(4w + 4)r + (4w + 4)s. (36)

Using Lemmas 1–3, we can translate the above formulas into the language of binomial coefficients and obtain:

THEOREM 1. For any positive natural number a and b, Syr(2a, b) holds if and only if there are natural numbers w, p, r, s and t such that $a \le w$, $b \le w$ and

$$\begin{pmatrix} 2w+1\\ w \end{pmatrix} \begin{pmatrix} p+r\\ p \end{pmatrix} \times \\ \begin{pmatrix} 4(w+1)(p+r)+1\\ p+r \end{pmatrix} \begin{pmatrix} pw\\ s \end{pmatrix} \begin{pmatrix} rw\\ t \end{pmatrix} \times \\ \begin{pmatrix} 2s+2t+r+b((4w+3)(p+r)+1)\\ 3((4w+4)t+a)+2(4w+4)r+(4w+4)s \\ 2s+2t+r+b((4w+3)(p+r)+1) \end{pmatrix} \times \\ \begin{pmatrix} 3((4w+4)t+a)+2(4w+4)r+(4w+4)s\\ 2s+2t+r+b((4w+3)(p+r)+1) \end{pmatrix} \equiv 1 \pmod{2}.$$

REMARK 1. We assume that $\binom{m}{n} = 0$ unless $0 \le n \le m$ and use this assumption for expressing the equality (36).

REMARK 2. Thanks to our special choice of w, conditions (29) and (30) can be written as

$$a \preceq w, \qquad b \preceq w \tag{37}$$

and hence can be replaced in the statement of the Theorem by two extra binomial coefficients. Another way to get rid of this inequalities would be to replace w everywhere by w + a + b.

2.4 Restatements of the 3x + 1 problem

We can obtain restatements of the 3x + 1 problem from Theorem 1 by substituting either b = 1 or b = 2. In the former case we get

COROLLARY 1. The 3x + 1 conjecture is true if and only if for every positive integer a there are natural numbers w, p, r, s and t such that $a \leq w$ and

$$\begin{pmatrix} 2w+1\\ w \end{pmatrix} \begin{pmatrix} p+r\\ p \end{pmatrix} \times \\ \begin{pmatrix} 4(w+1)(p+r)+1\\ p+r \end{pmatrix} \begin{pmatrix} wp\\ s \end{pmatrix} \begin{pmatrix} wr\\ t \end{pmatrix} \times \\ \begin{pmatrix} 2s+2t+r+(4w+3)(p+r)+1\\ 3((4w+4)t+a)+2(4w+4)r+(4w+4)s \\ 2s+2t+r+(4w+3)(p+r)+1 \end{pmatrix} \times \\ \begin{pmatrix} 3((4w+4)t+a)+2(4w+4)r+(4w+4)s\\ 2s+2t+r+(4w+3)(p+r)+1 \end{pmatrix} \equiv 1 \pmod{2}.$$

Substituting b = 2, we can further reduce the number of variable and binomial coefficients. Namely, in this case the equality from (36) allows us to give explicit expression of r in terms of the other variables:

$$r = 2t + 2(4w + 3)p + 2 - 3((4w + 4)t + a) - (4w + 2)s.$$
(38)

Substituting this value of r into other conditions we get

COROLLARY 2 The 3x + 1 conjecture is true if and only if for every positive integer number a there are natural numbers w, p, s and t such that $a \leq w$ and

$$\begin{pmatrix} 2w+1\\ w \end{pmatrix} \begin{pmatrix} wp\\ s \end{pmatrix} \times \\ \begin{pmatrix} p+2t+2(4w+3)p+2-3((4w+4)t+a)-(4w+2)s\\ p \end{pmatrix} \times \\ \begin{pmatrix} 4(w+1)(p+2t+2(4w+3)p+2-3((4w+4)t+a)-(4w+2)s)+1\\ p+2t+2(4w+3)p+2-3((4w+4)t+a)-(4w+2)s \end{pmatrix} \times \end{cases}$$

$$\begin{pmatrix} w(2t+2(4w+3)p+2-3((4w+4)t+a)-(4w+2)s)\\t \end{pmatrix} \equiv 1 \pmod{2}.$$

Note that if we fix the values of a, b, w and m satisfying (29)-(31), then there is at most one way to assing values to p, r, s and t satisfying (28) and (32)-(36). In order to avoid exponentiation, we would rather fix the value of v = p + r which, according to (28), uniquely determines m; we then eliminate pby substituting v - r for it. Now we can replace quantification over r, s and tby summation over the same variables:

COROLLARY 3. The 3x + 1 conjecture is true if and only if for every positive integer a there are natural numbers w and v such that $a \leq w$ and

$$\begin{pmatrix} 2w+1\\ w \end{pmatrix} \begin{pmatrix} 4(w+1)v+1\\ v \end{pmatrix} \sum_{r=0}^{\infty} \sum_{s=0}^{\infty} \sum_{t=0}^{\infty} \begin{pmatrix} v\\ r \end{pmatrix} \times \\ \begin{pmatrix} w(v-r)\\ s \end{pmatrix} \begin{pmatrix} wr\\ t \end{pmatrix} \times \\ \begin{pmatrix} 2s+2t+r+(4w+3)v+1\\ 3((4w+4)t+a)+2(4w+4)r+(4w+4)s\\ 2s+2t+r+(4w+3)v+1 \end{pmatrix} \times \\ \begin{pmatrix} 3((4w+4)t+a)+2(4w+4)r+(4w+4)s\\ 2s+2t+r+(4w+3)v+1 \end{pmatrix} \equiv 1 \pmod{2}.$$

REMARK 3. The triple sum, formally defined as infinite, is in fact finite thanks to "natural bounds": if r > v, s > w(v - r) or t > wr, then the corresponding binomial coefficient is equal to zero.

REMARK 4. Besides the above mentioned natural upper bounds for variables there is another important property which gives hope for successful application of summation technique from [15, 18], namely, the summation variables r, s and t come only linear.

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Appendix: Kummer's Theorem

THEOREM (Kummer [5]). If p is a prime number, then its exponent in the canonical expansion of the binomial coefficient $\begin{pmatrix} a+b\\a \end{pmatrix}$ into prime factors is

equal to the the number of carries required when adding the numbers a and b represented in the base p.

To prove this, note that the identity

$$\begin{pmatrix} a+b\\a \end{pmatrix} = \frac{(a+b)!}{a!\,b!} \tag{39}$$

implies that

$$v_p\left(\left(\begin{array}{c}a+b\\a\end{array}\right)\right) = v_p\left((a+b)!\right) - v_p(a!) - v_p(b!),\tag{40}$$

where $v_p(k)$ is the exponent of p in the prime factorization of k. It is not difficult to see that

$$v_p(k!) = \left\lfloor \frac{k}{p} \right\rfloor + \left\lfloor \frac{k}{p^2} \right\rfloor + \dots, \qquad (41)$$

because among the numbers 1, ..., k, there are exactly $\lfloor \frac{k}{p} \rfloor$ numbers divisible by p, exactly $\lfloor \frac{k}{p^2} \rfloor$ numbers divisible by p^2 , and so on. Thus,

$$v_p\left(\left(\begin{array}{c}a+b\\a\end{array}\right)\right) = \sum_{l\geq 1}\left(\left\lfloor\frac{a+b}{p^l}\right\rfloor - \left\lfloor\frac{a}{p^l}\right\rfloor - \left\lfloor\frac{b}{p^l}\right\rfloor\right).$$
(42)

Now it suffices to note that in this sum, the *l*th summand is equal to either 1 or 0, depending on whether or not there is a carry from the (l-1)th digit.

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