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A binomial representation of the $3x + 1$ problem

by

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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:

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

Consider further its iteration g defined recursively as

$$g(a,0) = a, \qquad g(a,k+1) = f(g(a,k)), \tag{2}$$

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

$$\mathrm{Syr}(a,b) \;\Leftrightarrow\; \exists m\; g(a,m) = b. \tag{3}$$

We say that a number m such that $g(a,m) = b$ *realizes* $\mathrm{Syr}(a,b)$, 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 $\mathrm{Syr}(a,1)$ holds and hence the sequence of iterated values a, $f(a)$, $f(f(a))$, $\ldots$ eventually becomes periodic: $\ldots,1,2,1,2,1,2,\ldots$ 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 a more recent paper [10].

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1.2. *The language of binomial expressions*. In the first half of the XX century the process of formalization of mathematics reached some culminating point thanks to Gödel [3] who showed that many mathematical statements can be expressed by arithmetical formulas, i.e. by formulas of the form

$$\mathrm{Q}_1\, x_1\, \mathrm{Q}_2\, x_2\, \ldots\, \mathrm{Q}_k\, x_k\, G(x_1, x_2, \ldots, x_k) \tag{4}$$

where the Q's are universal or existential quantifiers, the 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 the arithmetical operations of addition, subtraction and multiplication, the relation of equality and the logical operations AND, OR and NOT.

About forty years later, Davis–Matiyasevich–Putnam–Robinson established the negative answer to Hilbert's tenth problem, by proving that if all the universal quantifiers 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

$$\exists\, x_1\, \exists\, x_2\, \ldots\, \exists\, x_m\, P(x_1, \ldots, x_m) = 0 \tag{5}$$

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 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 at the intermediate steps in transformation of (4) into (5) starting from the 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 arithmetical formula containing only operations of addition, subtraction and multiplication.

Second, when congruence with fixed modulus is used as the predicate symbol instead of the equality relation (as in Theorem 1 below), the existential quantifiers can, under some conditions, be replaced by summation (as in Corollary 3 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 examples 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 identity found can be feasible for a human being, which opens new ways to attacking 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 surprisingly 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. Earlier examples are the Mann–Shanks [9] criterion of primality in terms of divisibility of several binomial coefficients and the second author's 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 using 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. *Preliminary tools.* Let a, b be natural numbers (by which we understand non-negative integers). Their binary representations 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 with 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:

$$a \preceq b \;\Leftrightarrow\; \forall i\ \alpha_i \le \beta_i, \tag{6}$$

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

As an example, take

$$\begin{array}{cl} c & 1\,0\,0\,1\,1\,0\,0\,1 \\ b & 1\,0\,0\,1\,0\,0\,0\,1 \\ a & 1\,0\,0\,0\,1\,0\,0\,1 \end{array}$$

Here $a \preceq c$, $b \preceq c$ but $a \not\preceq b$.

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*

$$a \preceq b \;\Leftrightarrow\; \binom{b}{a} \equiv 1 \pmod 2. \tag{7}$$

Proof. The lemma follows immediately from a theorem due to Kummer [5] (for modern presentation see, for example, [16]). For completeness, a proof of Kummer's theorem is given in the appendix. ∎

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

$$a \perp b \;\Leftrightarrow\; \forall i\ \alpha_i\beta_i = 0 \;\Leftrightarrow\; \sum_i \alpha_i\beta_i = 0. \tag{8}$$

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

Lemma 2. *For any natural numbers a and b, $a \perp b$ if and only if $a \preceq a+b$.*

P r o o f. 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 $\perp$ the property of being 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 $u \preceq (4w+4)u+1$.*

P r o o f. The binary notation of a number u of the required form looks like

$$1\,\underbrace{0\ldots0}_{k+1}\,1\,\underbrace{0\ldots0}_{k+1}\,1\ \ldots\ 1\,\underbrace{0\ldots0}_{k+1}\,1 \tag{9}$$

and is completely characterized by the following properties:

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

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

2.2. *Representations of finite sequences.* Consider a finite sequence of natural numbers

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

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

$$x_i < 4w+4, \quad i = 1, \ldots, m. \tag{11}$$

We shall say that the number

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

w-represents the sequence (10) or is the *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, with leading zeros to the length $k+2$.

Here is an example: the binary notation of the number which 31-represents the sequence $\langle 18, 9, 14, 7 \rangle$ is

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

We see that the 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 the number (12) *strongly w-represents* the sequence (10) or is the *strong w-representation* of (10) if the following condition (stronger than (11)) is satisfied:

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

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

Define four functions $\pi, \varrho, \sigma, \tau$ on the natural numbers in the following way: if $x = 2z + y$ with $y \in \{0, 1\}$, then

$$\pi(x) = 1 - y, \qquad \varrho(x) = y,$$
$$\sigma(x) = (1-y)z, \qquad \tau(x) = yz.$$

The functions π and ϱ determine 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 on the parity of x. Accordingly, for every x,

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

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:

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

We shall use the following notation: if φ is a function from $\mathbb{N}$ into $\mathbb{N}$ then

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

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

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

Q	0000111 0001110 0001001 0010010
P	0000000 0000001 0000000 0000001
R	0000001 0000000 0000001 0000000
S	0000000 0000111 0000000 0001001
T	0000011 0000000 0000100 0000000

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

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

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

Note that F need not be a strong representation, however, the condition (14) implies that $f(x_i) < 4w + 4$, as required by 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 going to state a condition which is necessary and sufficient for these numbers to form the detailed w-representation of some sequence (10).

First of all, p and r should be orthogonal:

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

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

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

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

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

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

Summing up, we get

LEMMA 5. *Let $w + 1$ be a power of 2. Then four numbers p, r, s, and t form the 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 ourselves to even initial numbers, i.e., the $3x+1$ problem can be stated as $\forall a\, \mathrm{Syr}(2a,1)$ and as $\forall a\, \mathrm{Syr}(2a,2)$. Suppose now that some positive integer m realizes $\mathrm{Syr}(2a,b)$ for given a and b. This means that the equation

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

has a solution

$$x_i = g(2a, i), \quad i = 1, \ldots, m-1. \tag{23}$$

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

If $w+1$ is a power of 2 so high 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 the numbers

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

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), the 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,

$$b \le w, \tag{25}$$

then the sequence from the right-hand side of (22) is w-represented by the number $2(s+t)+r+(4w+4)^{m-1}b$. Thus we can rewrite (22) as

$$\begin{aligned} 2(s+t) + r + (4w+4)^{m-1}b \\ = 3((4w+4)t+a) + 2(4w+4)r + (4w+4)s. \end{aligned} \tag{26}$$

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

$$(4w+4)^{m-1} = (4w+3)(p+r) + 1. \tag{28}$$

We can now sum up our argument in

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

$$a \le w, \tag{29}$$

$$b \le w, \tag{30}$$

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

$$p \perp r, \tag{32}$$

$$p+r \preceq 4(w+1)(p+r)+1, \tag{33}$$

$$s \preceq pw, \tag{34}$$

$$t \preceq rw, \tag{35}$$

$$\begin{aligned} 2s+2t+r+b((4w+3)(p+r)+1) \\ = 3((4w+4)t+a)+2(4w+4)r+(4w+4)s. \end{aligned} \tag{36}$$

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

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

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

Remark 1. We assume that $\binom{m}{n}=0$ unless $0 \le n \le m$ and use this assumption when translating 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 these 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 $a \le w$*

and

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

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

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

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* $a \le w$ *and*

$$\binom{2w+1}{w}\binom{wp}{s}$$
$$\times\binom{p+2t+2(4w+3)p+2-3((4w+4)t+a)-(4w+2)s}{p}$$
$$\times\binom{4(w+1)(p+2t+2(4w+3)p+2-3((4w+4)t+a)-(4w+2)s)+1}{p+2t+2(4w+3)p+2-3((4w+4)t+a)-(4w+2)s}$$
$$\times\binom{w(2t+2(4w+3)p+2-3((4w+4)t+a)-(4w+2)s)}{t}\equiv 1 \pmod 2.$$

Note that if we fix the values of a, b, w and m satisfying (29)–(31), then there is at most one way to assign 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 p by substituting $v - r$ for it. Now we can replace quantification over r, s and t by 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* $a \le w$ *and*

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

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 zero.

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

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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 $\binom{a+b}{a}$ into prime factors is equal to the number of carries required when adding the numbers a and b represented in base p.*

To prove this, note that the identity

$$\binom{a+b}{a} = \frac{(a+b)!}{a!\,b!} \tag{39}$$

implies that

$$v_p\left(\binom{a+b}{a}\right) = v_p((a+b)!) - v_p(a!) - v_p(b!), \tag{40}$$

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

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

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

$$v_p\left(\binom{a+b}{a}\right) = \sum_{l\ge 1}\left(\left\lfloor\frac{a+b}{p^l}\right\rfloor - \left\lfloor\frac{a}{p^l}\right\rfloor - \left\lfloor\frac{b}{p^l}\right\rfloor\right). \tag{42}$$

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

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