Unsolved Problems In Computational Science

Part Two

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Work in Progress

About the tile: Unsolved Problems In Computational Science: Part Two

I submitted a paper “Challenging Problems in Discrete Mathematics”
to a conference
 “The 2014 World Congress in Computer Science, Computer Engineering, and Applied computing”
The Conference paper acceptance rate: 23%

Referee report:
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(3) This is an excellent paper.
(4) Recommend: accept.
(5) Suggestion: Use the first 7 pages for this conference.
(6) Suggestion: Change the tile to “Unsolved Problems In Computational Science: Part One “.
For the remaining 10 pages, you could use the title “Unsolved Problems In Computational Science: Part Two/Part Three” for the next conference or other conference or journals.

A self-avoiding walk (SAW) is a sequence of moves on a lattice not visiting the same point more than once.

Problem

What is the number of SAWs from $(0,0)$ to $(n-1,n-1)$ in an $n \times n$ grid, taking steps from $\{\uparrow,\downarrow,\leftarrow,\rightarrow\}$?

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Donald Knuth claimed that the number is between 1.3×10^{24} and 1.6×10^{24} for $n = 11$ and he did not believe that he would ever in his lifetime know the exact answer to this problem in 1975.

Is Knuth's claim true?

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Is Knuth's claim true?

Richard Schroeppel pointed out that the exact value is

$$
\begin{aligned}
&15687580304647500132141 00 \\
&= 2^2 3^2 5^2 31 \times 115\,422\,379 \times 487\,148\,912\,401 \\
&= 1.\,568\,8 \times 10^{24}
\end{aligned}
$$

It is still an unsolved problem for $n > 25$.

Problem

What is the number $f(n)$ of n-step SAWs, on the square lattice, taking steps from $\{\uparrow, \downarrow, \leftarrow, \rightarrow\}$?

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$$2^n \leq f(n) \leq 4 \times 3^{n-1}$$

$$f(m+n) \leq f(m) f(n)$$

There exists a constant C such that

$$\lim_{n \to \infty} f(n)^{1/n} = C.$$

$C = 2.64$ (up to 71 steps have been counted).

$C = 2.638$ (up to 91 steps have been counted).

$$f(n) \approx 2.638^n$$

The number of SAWs/ the number of total walks:

$\frac{1}{1200}$ for $n = 20$

$\frac{1}{2.4 \times 10^8}$ for $n = 50$

Prudent self-avoiding walks:

A PSAW is a proper subset of SAW on the square lattice. The walk starts at $(0,0)$, and the empty walk is a PSAW. A PSAW grows by adding a step to the end point of a PSAW such that the extension of this step - by any distance - never intersects the walk. Hence the name prudent. The walk is so careful to be self-avoiding that it refuses to take a single step in any direction where it can see - no matter how far away - an occupied vertex.

A.J. Guttmann, E. Duchi, P. Préa, T.M. Garoni, I. Jensen and J.C. Dethridge.

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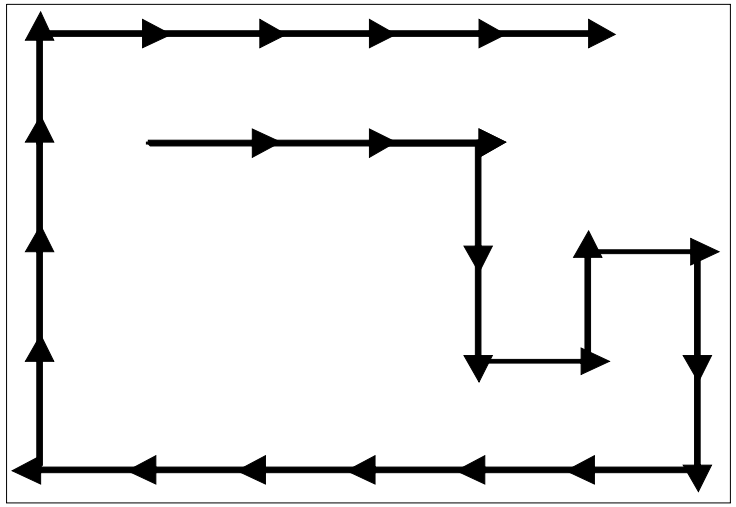
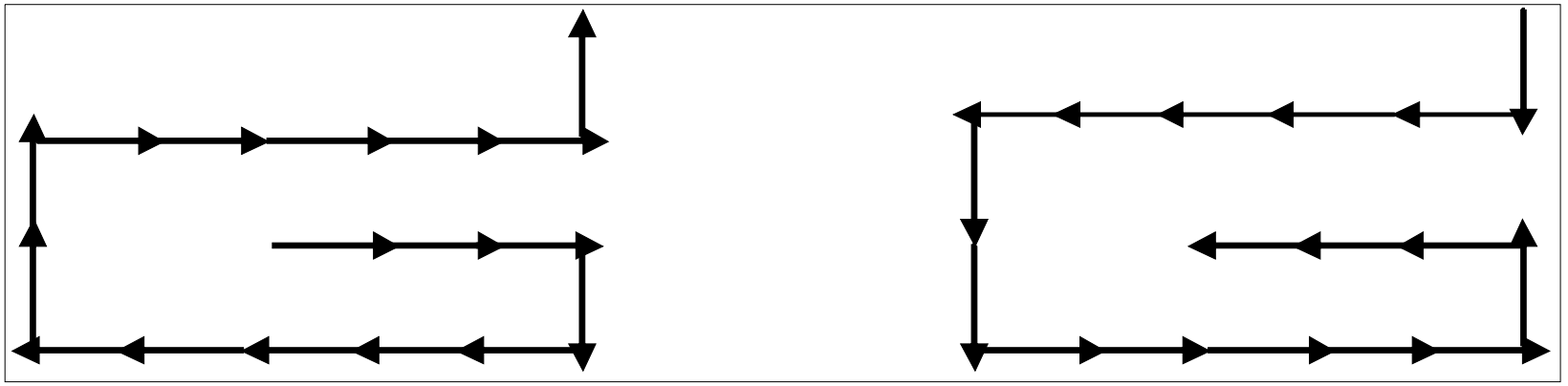


Properties of a PSAW

Unlike SAW, PSAW are usually not reversible.



Each PSAW possesses a minimum bounding rectangle, which we call *box*.

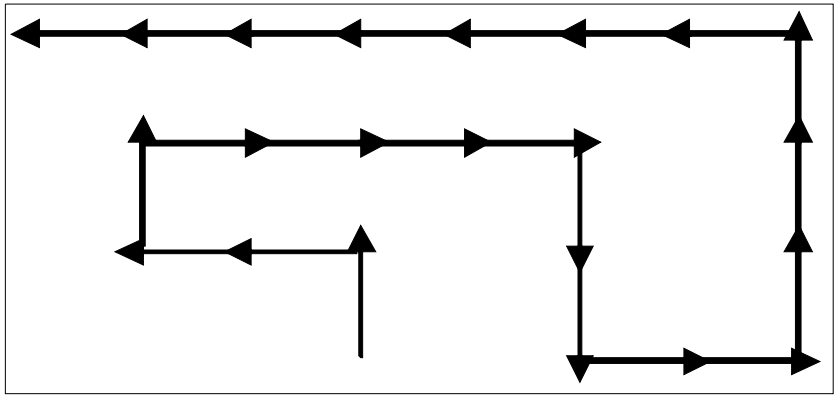
The endpoint of a prudent walk is always a point on the boundary of the box.

Each new step either inflates the box or walks (prudently) along the border.

After an inflating step, there are 3 possibilities for a walk to go on. Otherwise, only 2.

In a *one-sided* PSAW, the endpoint lies always on the top side of the box. The walk is *partially directed*.

A prudent walk is *two-sided* if its endpoint lies always on the top side, or on the right side of the box.



One-sided PSAWs

What is the number (say $f(n)$) of one-sided n-step prudent walks, taking steps from $\{\uparrow, \leftarrow, \rightarrow\}$?

The generating function equals

$$\sum_{n \geq 0} f(n)t^n = \frac{1+t}{1-2t-t^2} = 1 + 3t + 7t^2 + 17t^3 + 41t^4 + 99t^5 + 239t^6 + \ldots$$

Also,

$$\begin{aligned} f(n) &= 2f(n-1) + f(n-2) \\ &= \frac{(1-\sqrt{2})^n + (1+\sqrt{2})^n}{2} \\ &= \begin{bmatrix} 1 & 0 \end{bmatrix} \left(\sum_{k=0}^{n+1} \binom{n+1}{k} \begin{bmatrix} 0 & 1 \\ 2 & 0 \end{bmatrix}^k \right) \begin{bmatrix} 1 \\ 0 \end{bmatrix}. \end{aligned}$$

We obtain sequence $A001333$ of the On-Line Encyclopedia of Integer Sequences.

What is the number of the one-sided n-step prudent walks, avoiding k or more consecutive east steps, $\rightarrow^{\geq k}$?

The generating function equals

$$\frac{1+t-t^k}{1-2t-t^2+t^{k+1}}$$

If $k=2$, we obtain sequence $A006356$, counting the number of paths for a ray of light that enters two layers of glass and then is reflected exactly n times before leaving the layers of glass.

If $k=3$, we obtain sequence $A033303$.

What is the number of one-sided n-step prudent walks in the first quadrant, starting from $(0,0)$ and ending on the y-axis, taking steps from $\{\uparrow,\leftarrow,\rightarrow\}$?

The generating function is

$$\frac{1}{2t^3}((1+t)(1-t)^2-\sqrt{(1-t^4)(1-2t-t^2)}\,).$$

What is the number of one-sided n-step prudent walks *exactly* avoiding $\leftarrow^{=k}$, taking steps from $\{\uparrow, \leftarrow, \rightarrow\}$?

The generating function equals

$$\frac{1 + t - t^k + t^{k+1}}{1 - 2t - t^2 + t^{k+1} - t^{k+2}}.$$

If $k = 1,$ we obtain sequence $A078061$.

What is the number of one-sided n-step prudent walks exactly avoiding $\leftarrow^{=k}$ and $\uparrow^{=k}$ (both at the same time)?

The generating function is

$$\frac{1+t-2t^k+2t^{k+1}}{1-2t-t^2+2t^{k+1}-2t^{k+2}}.$$

For $k=1$,

$$f(n) = (2^{n+2} - (-1)^{\lfloor n/2 \rfloor} + 2(-1)^{\lfloor (n+1)/2 \rfloor})/5,$$

also,

$$f(n) = 2f(n-1) - f(n-2) + 2f(n-3)$$

with $f(1) = 1, f(2) = 3, f(3) = 7.$

This is sequence $A007909$.

Two-sided PSAWs

What is the number of two-sided, n-step prudent walks ending on the top side of their box avoiding both patterns $\leftarrow^{\geq 2}$, $\downarrow^{\geq 2}$ (both at the same time), taking steps from $\{\uparrow, \downarrow, \leftarrow, \rightarrow\}$?

Two-sided PSAWs

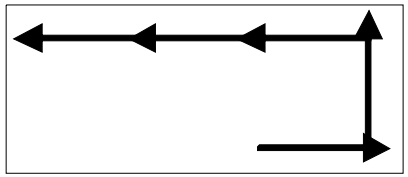
What is the number of two-sided, n-step prudent walks ending on the top side of their box avoiding both patterns $\leftarrow^{\geq 2}$, $\downarrow^{\geq 2}$ (both at the same time), taking steps from $\{\uparrow, \downarrow, \leftarrow, \rightarrow\}$?

Theorem *The generating function (say $T(t,u)$) of the above two-sided prudent walks ending on the top side of their box satisfies*

$$\left(1 - t^2u - \frac{tu}{u-t}\right)T(t,u) = 1 + tu + T(t,t)t\frac{u-2t}{u-t},$$

where u counts the distance between the endpoint and the north-east (NE) corner of the box.

A walk takes 5 steps, and the distance between the endpoint and the north-east corner is 3. So we can use t^5u^3 to count this walk.



Solve this generating function for $T(t,u)$ using the Kernel Method:

From

$$\left(1 - t^2u - \frac{tu}{u-t}\right)T(t,u) = 1 + tu + T(t,t)\left(t - \frac{t^2}{u-t}\right),$$

we can get

$$\begin{aligned}&(1-tu)(u-tu-t-t^2u^2+t^3u)T(t,u)\\ &= (u-t)(1-tu)(1+tu) - T(t,t)(1-tu)t(2t-u)\end{aligned}$$

Set $(1-tu)(u-tu-t-t^2u^2+t^3u) = 0$, then there is only one *power series* solution for u

$$u = \frac{1}{2t^2}\left(1 - t + t^3 - \sqrt{(1-t-t^3)^2 - 4t^4}\right).$$

Set

$$(1+tu)(u-t)(1-tu)+T(t,t)(1-tu)t(u-2t)=0,$$

and replace u by U:

$$T(t,t)=(1+tU)\frac{t-U}{t(U-2t)}.$$

From

$$\begin{aligned}&(1-tu)(u-t-tu-t^2u^2+t^3u)T(t,u)\\&=(u-t)(1-tu)(1+tu)-T(t,t)(1-tu)t(2t-u)\end{aligned}$$

get

$$T(t,u)=\frac{(t-u)(1-tu)(1+tu)+T(t,t)(1-tu)t(2t-u)}{(1-tu)(u-t-tu-t^2u^2+t^3u)}.$$

Replace $T(t,t)$ by $T(t,t) = (1+tU)\frac{t-U}{t(U-2t)}$.

$$T(t,u) = \frac{(1+tu)(u-t)}{u-t-tu-t^2u^2+t^3u} - \frac{(1+tU)(U-t)(1-tu)(u-2t)}{(U-2t)(1-tu)(u-t-tu-t^2u^2+t^3u)}$$

Notice that $T(t,1)$ is the generating function of the number of two-sided n-step prudent walks ending on the top side of their box avoiding both patterns $\leftarrow^{\geq 2}$, $\downarrow^{\geq 2}$, taking steps from $\{\uparrow,\downarrow,\leftarrow,\rightarrow\}$, thus $T(t,1) =$

$$\frac{(1-2t)(1-t)\sqrt{(1-t-t^3)^2-4t^4}-(1+t)(1-7t+14t^2-11t^3+10t^4-4t^5)}{2t(1-2t-t^2+t^3)(1-2t-2t^3)}$$

$$= 1+3t+6t^2+15t^3+35t^4+83t^5+195t^6+460t^7+1085t^8+\ldots$$

Note that $T(t,0)$ is the generating function of the number of two-sided n-step prudent walks ending at the north-east corner of their box avoiding both patterns $\leftarrow^{\geq 2}$, $\downarrow^{\geq 2}$, taking steps from $\{\uparrow,\downarrow,\leftarrow,\rightarrow\}$, so $T(t,0) =$

$$\frac{(1-t)\sqrt{(1-t-t^3)^2-4t^4}\ -1+3t-t^2+t^3+t^4}{(1-2t-2t^3)t}$$

$$= 1+2t+4t^2+10t^3+24t^4+56t^5+130t^6+304t^7+714t^8+1678t^9+\ldots$$

Furthermore, $2T(t,1) - T(t,0)$ is the generating function of the number of two-sided n-step prudent walks ending on the top side or right side of their box avoiding both patterns $\leftarrow^{\geq 2}$, $\downarrow^{\geq 2}$, taking steps from $\{\uparrow, \downarrow, \leftarrow, \rightarrow\}$, thus

$$2T(t,1) - T(t,0) =$$

$$\frac{t(1-t)^2\sqrt{(1-t-t^3)^2 - 4t^4} + 1 - t - 2t^2 - 2t^3 - 2t^4 + 4t^5 - t^6}{(1-2t-t^2+t^3)(1-2t-2t^3)}$$

$$= 1 + 4t + 8t^2 + 20t^3 + 46t^4 + 110t^5 + 260t^6 + 616t^7 + 1456t^8 + 3442t^9 + \ldots$$

Open Problem 1

What is the number of two-sided n-step prudent walks, ending on the top side of their box, avoiding both $\leftarrow^{\geq k}$, and $\downarrow^{\geq t}$ ($k \neq t$) taking steps from $\{\uparrow, \downarrow, \leftarrow, \rightarrow\}$?

Open Problem 2

What is the number of two-sided n-step prudent walks, ending on the top side of their box, exactly avoiding both $\leftarrow^{=k}$, $\downarrow^{=t}$ ($k, t \geq 3$), taking steps from $\{\uparrow, \downarrow, \leftarrow, \rightarrow\}$?

Let $f(m,n)$ be the number of paths from $(0,0)$ to (n,n) avoiding $\uparrow^{\geq k}$ and $\rightarrow^{\geq k}$,taking steps from $\{\uparrow, \rightarrow\}$. Then

$$f(m,n) = f(m-1,n) + f(m,n-1) - f(m-k,n-1) - f(m-1,n-k) + f(m-k,n-k).$$

For $k = 3,$ using finite operator calculus:

$$\frac{(1-t)^2\sqrt{(1+t+t^2)(1-3t+t^2)} - (1-3t+t^2)(1+t^2)}{t^2(1-3t+t^2)}$$

$$= 2t + 6t^2 + 14t^3 + 34t^4 + 84t^5 + 208t^6 + 518t^7 + \ldots .$$

This solved a conjecture of R. Stephan

Markoff equation $x^2+y^2+z^2=3xyz$

Positive integer solutions:

1, 1, 1

2, 1, 1

5, 2, 1

Markoff equation $x^2+y^2+z^2=3xyz$

Positive integer solutions:
1, 1, 1
2, 1, 1
5, 2, 1

$x^2+y^2+z^2=xyz$
3, 3, 3
6, 3, 3
15, 6, 3

Markoff equation $x^2+y^2+z^2=3xyz$

Positive integer solutions:
1, 1, 1
2, 1, 1
5, 2, 1

$x^2+y^2+z^2=xyz$
3, 3, 3
6, 3, 3
15, 6, 3

Does $x^2+y^2+z^2=2xyz$ have positive integer solution?

$$x_1^2+x_2^2+\ldots+x_n^2 = kx_1x_2\ldots x_n \qquad (1)$$

k positive integer
$n \geq 3$
Positive integer solutions
Markoff-Hurwitz equation
generalized Markoff equation.

$$x_1^2+x_2^2+\ldots+x_n^2 = kx_1x_2\ldots x_n \qquad (1)$$

k positive integer
$n \geq 3$
Positive integer solutions
Markoff-Hurwitz equation
generalized Markoff equation.

When does equation (1) have solution?

$$x_1^2+x_2^2+\ldots+x_n^2 = kx_1x_2\ldots x_n \qquad (1)$$

k positive integer
$n\geq 3$
Positive integer solutions
Markoff-Hurwitz equation
generalized Markoff equation.

When does equation (1) have solution?

$n=k$, $x_1=x_2=\ldots=x_n=1$

If $x_1, x_2, \ldots, x_n$ is a solution to equation (1), then
$x_1, x_2, \ldots, x_{i-1}, kx_1x_2 \ldots x_{i-1}x_{i+1} \ldots x_n - x_i, x_{i+1}, \ldots, x_n$
is also a solution (for each $1 \leq i \leq n$).

$x^2+y^2+z^2=3xyz$

1, 1, 1

2, 1, 1

Equation (1) does not have solutions when k>n for n≥2.
A. Hurwitz 1907, S.Gao 2005

The American Mathematical Monthly, Vol. 117, No. 6 (June-July 2010):

An Old Four-Squares Chestnut

11374 [2008, 568]. *Proposed by Harley Flanders and Hugh L. Montgomery, University of Michigan, Ann Arbor, MI.* Let a, b, c, and m be positive integers such that $abcm = 1 + a^2 + b^2 + c^2$. Show that $m = 4$.

Solution by Afonso Bandeira and Joel Moreira, Universidade de Coimbra, Portugal, and João Guerreiro, Instituto Superior Técnico, Portugal. Viewing the equation modulo 4 shows that 4 divides m. Let $n = m/4$. Now suppose there is a solution with $n > 1$. Let (a, b, c) be such a solution where $a + b + c$ is minimal. Name the values so that $a \geq b \geq c$.

Now a is a solution to the quadratic equation $x^2 - x(4bcn) + (b^2 + c^2 + 1) = 0$. By Vieta's formula, another solution is a', where $a' = 4bcn - a$. If $a' \geq a$, then $a^2 + b^2 + c^2 + 1 = 4abcn \geq 2a^2$, and so $a^2 \leq b^2 + c^2 + 1 \leq 2b^2 + 1$. Now $a^2 < a^2 + 1 \leq 2b^2 + 2 \leq 4b^2$, so $a < 2b$. This yields $4abcn > 2a^2cn \geq 4a^2 \geq a^2 + b^2 + c^2 + 1$, which contradicts (a, b, c) being a solution.

Thus (a', b, c) is a solution that contradicts the minimality of $a + b + c$. We conclude that $n > 1$ is impossible, so $n = 1$ and $m = 4$.

Editorial comment. We print this proof because of its brevity. A. Hurwitz showed in Über eine Aufgabe der unbestimmten Analysis, *Arch. Math. Phys.* **3** (1907) 185–196, that $x_1^2 + x_2^2 + \cdots + x_n^2 = kx_1x_2 \ldots x_n$ has no solution in positive integers if $k > n$, from which the present claim follows directly. This reference was supplied by each of S. Gao, W. C. Jagy, J. H. Jaroma, and J. P. Robertson. A new proof of Hurwitz's theorem may be found in S. Gao, C. Caliskan, and S. Rong, Some properties of n-dimensional generalized Markoff equation, *Congr. Numer.* **177** (2005) 217–221.

Also solved by R. Chapman (U.K.), J. Christopher, P. Corn, S. Gao, H. S. Hwang & K. J. Kim (Korea), I. M. Isaacs, W. C. Jagy, J. H. Jaroma, O. Kouba (Syria), O. P. Lossers (Netherlands), É. Pité (France), C. R. Pranesachar (India), J. P. Robertson, B. Schmuland (Canada), N. C. Singer, R. Stong, H. T. Tang, M. Tetiva (Romania), Fisher Problem Group, Szeged Problem Solving Group "Fejéntaláltuka" (Hungary), GCHQ Problem Solving Group (U.K.), Microsoft Research Problems Group, NSA Problems Group, and the proposers.

We call a solution $x_1, x_2. ..., x_n$ of (1) an ordered solution if $x_1 \geq x_2 \geq ... \geq x_{n.}$

Let $x_i' = kx_1x_2...x_{i-1}x_{i+1}...x_n - x_{i.}$, we know if $x_1, x_2, ..., x_i, ..., x_n$ form a solution of (1) then $x_1, x_2, ..., x_i', ..., x_n$ also form a solution. We say the new solution comes from the original solution on index i.

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Lemma 1. Let X: $x_1, x_2, ..., x_i, ..., x_n$ be an ordered solution and $i \geq 2$. Then
$x_i' = kx_1x_2...x_{i-1}x_{i+1}...x_n - x_i > x_1$.

Definition Let X: $x_1, x_2, ..., x_i, ..., x_n$ and Y; $y_1, y_2, ..., y_i, ..., y_n$ be two ordered solutions of (1). We define X < Y (X comes before Y in lexical order) iff there exists i such that $1 \leq i \leq n$ and $x_j = y_j$ for $1 \leq j < i$ and $x_i < y_i$. We say X is the minimum solution if X < Y for any other solution Y of (1).

If equation (1) has one solution then it has infinitely many solutions.

It is very tough to find a solution to equation (1) for some n and k.

Algorithm 1 Systematic Search for Solutions
// Check all possible ordered solutions with each
// component $1 \leq x[i] \leq$ Limit
// The average time complexity is about O ($Limit^2$), since the cut-offs usually occur at early stages when i = 2 or 3

We implemented the Algorithm 1 and ran on a half dozen PCs of Intel Core i7-2600K Quad-Core Processor 3.4 Ghz or equivalent for n = 3, 4,…, 9 and k = 1, 2,…, n. The Limit was set to 1,000,000. Each (n, k) case used a single thread. A PC ran up to 8 cases simultaneously. The timing data in hours have been converted to that of Intel Core i7-2600K 3.4 Ghz for comparison. We summarized the results for n = 3, 4, …, 9.

	Limit 1,000,000	N = 7	N = 8	N = 9
K = 1	#Ord. Solutions	124	61	0
	Min. Solution	3, 2, 2, 2, 1, 1, 1	4, 2, 2, 2, 1, 1, 1	No
	Proc. Time in hrs	279.95	356.11	376.87
k = 2	#Ord. Solutions	64	0	0
	Min. Solution	2, 2, 2, 1, 1, 1, 1	No	No
	Proc. Time in hrs	122.4	153.1	162.9

There are no solutions with all $x_i \leq 1{,}000{,}000$ for (n, k) cases:
(3, 2), (4, 2), (4, 3), (5, 2), (5, 3), (6, 1), (6, 2), (6, 4), (6, 5),
(7, 4), (7, 6), (8, 2), (8, 3), (8, 4), (8, 5), (8, 6), (8, 7), (9, 1),
(9, 2), (9, 3), (9, 4), (9, 5), (9, 7), (9, 8).

Algorithm 2 Generating Solutions

We use Algorithm 1 to find the minimum solution M (within the limit). If the minimum solution is found, we use Algorithm 2

The time complexity of Algorithm 2 is $O(s^2)$ where s is the number of ordered solutions within the limit when case (n, k) has solutions, the same as Algorithm 1 when there is no solutions. Algorithm 2 is several order of magnitude faster than Algorithm1 when solutions exist. When we used 1,000,000 as the value limit, this algorithm took just a small fraction of a second to solve equation (1) (if there is a solution) when Algorithm 1 had taken days.

We have proved mathematically that solutions to equation (1) do not exist for (n, k) = (3, 2), (4, 2), (4, 3), (5, 2), (5, 3) after the computer couldn't find any solutions limited to 1,000,000.

Does $x^2+y^2+z^2=2xyz$ have positive integer solution?

Given n & k, the leading term of the ordered solutions of equation (1) in non-decreasing order form an integer sequence if the solutions exist. So far we have not found same leading term from two different ordered solutions for a given (n, k).

n=3 and k=3
Solutions:
1, 1, 1,
2, 1, 1,
5, 2, 1,
13, 5, 1,
29, 5, 2,
34, 13, 1,
Sequence for n=3 and k=3:
1,2,5,13,29,34,89,169,194,233,433,610,985,...
The number of distinct prime divisors of any of the first 93 terms is less than 6. The second, third, 4th, 5th, 6th, 10th, 11th, 15th, 16th, 18th, 20th, 24th, 25th, 27th, 30th, 36th, 38th, 45th, 48th, 49th, 69th, 79th, 81th, 86th, 91th terms are primes.

The Online Encyclopedia of Integer Sequences http://oeis.org

Conjecture 1

Given (n, k), any ordered solution S of equation (1) can be generated from the minimum ordered solution M using the component replacement method in a finite number of steps.

Conjecture 2

If x_1, x_2. ..., x_n and x_1', x_2'. ..., x_n' are two different ordered solutions of (1) then $x_1 != x_1'$.

Conjecture 3

For $(n, k) = (6, 1), (6, 2), (6, 4), (6, 5), (7, 4), (7, 6), (8, 2), (8, 3), \ldots, (8, 7), (9, 1), \ldots, (9, 5), (9, 7), (9, 8)$, equation (1) has no solutions

Conjecture 4

The minimum solution of (1) consists of at least a 1 for $n \geq 5$.

Conjecture 4 is true for all the minimum solutions that we have found for $5 \leq n \leq 20$.

Conjecture 5

The leading term in the minimum ordered solution of (1) is not greater than n for $n \geq 3$.

The maximum leading term among all the minimum solutions of (1) that we have obtained is 5 for $3 \leq n \leq 20$.

Conjecture:

Let $p \neq 5$ be a prime, then

$\{2,4,6,..,p-3\} \subset \{\binom{p-1}{a_1}\binom{a_1-1}{a_2}\binom{a_2}{a_3}\binom{a_3}{a_4}\ldots\binom{a_{n-1}}{a_n} \bmod p : a_i$ is a positive integer, $p-1 \geq a_1,\ a_1 - 1 > a_2 > a_3 > a_4 > \ldots > a_n\}$.

We can prove that this conjecture is true for $p > 10^{30}$.

We can verify this conjecture is true for some small p, for instance $p < 10^7$.

Thank you for attending!

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