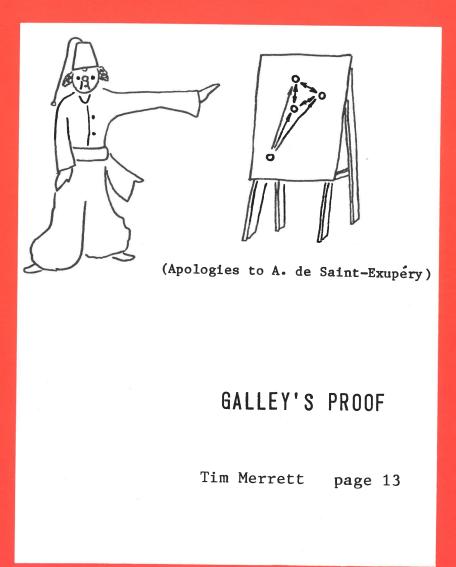
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Counting the Number of Isomeres of an Alkane with a Given Number of Carbon-Atoms

Hans Kummer

[Hans Kummer is Associate Professor in the Department of Mathematics and Statistics at Queen's. This article is based on a talk he gave this past year to the Undergraduate Math Club. Many hours of fine and fruitful exploration can emerge from the tree-counting problems that arise here, for students, teachers and parents alike. Read as much of it as you need to get going, then dip into the rest as you require.]

Alkanes are hydrocarbons with the molecular formula CH_{n-2n+2} where n is some natural number. For n = 1 we obtain CH_{4} which is the molecular formula of methane, an odourless gas which is the major component of natural gas. For n = 3 we obtain CH_{3} , the molecular formula of the well-known propane gas used nowadays by economy-minded individuals to fuel their cars.

The molecular formula of a compound does not give any information about the way the individual atoms are linked together to form the basic building block of the compound: The molecule. It is the <u>structural formula</u> which expresses this information. For instance the structural formula of methane is given by the diagram:

and the structural formula of propane is:

In these formulae the following two basic valency laws of Chemistry are reflected: The C-atom has valency 4, i.e. there are 4 valency strokes incident at each C-atom; similarly the hydrogen atom has valency 1 and hence there is precisely one valency stroke incident at each hydrogen atom.

In the cases n=1 (methane), n=2 (ethane) and n=3 (propane) the molecular formula together with the valency laws does uniquely determine the structural formula of the alkane. However in the case n=4 (butane) this is no longer the case. In fact there are two butanes (compounds with the molecular formula $\begin{pmatrix} C & H \\ 4 & 10 \end{pmatrix}$ whose respective structural formulae are:

The chemists describe the situation by saying that butane has two <u>isomeres</u>, the normal butane (n-butane) and the isobutane. The two compounds are easily distinguishable by their respective physical properties; e.g. n-butane has a boiling point of -0.5 C whereas isobutane already boils at -10.2 C.

As the number n of C-atoms increases, the number of isomeres of the corresponding alkane increases rapidly. The following table does illustrate this point quite vividly.

Name of alkane	u = # of C-atoms	Number of isomeres
and the second second		
methane	1	1
ethane	2	1
propane	3	1
butane	4	2
pentane	5	3
hexane	6	5
heptane	7	9
octane	8	18
nonane	9	35
decane	10	75

The problem, how to compute the number of isomeres of the alkane with a given number of C-atoms, is a famous combinatorial problem whose complete solution was given by George Polya in 1937 in a beautifully written paper. 1)

By studying his solution we learn a great deal about the methods which mathematicians employ in order to elucidate a complicated situation. Among these methods the method of <u>abstraction</u> ranks very high. It is characterized by disregarding details which are irrelevant for the problem under consideration.

Looking at the structural formulae of butane and isobutane we may first disregard the H-atoms and focus our attention only on the C-atoms.

$$C-C-C$$
 $C-C$

It is clear that we easily can recover the structural formulae by adding to each C as many H's as to restore the valency four of each C-atom and then draw valency strokes from the H-atoms to the corresponding C-atoms. We can go further in our process of abstraction by representing the C-atoms simply by points



In this way we arrive at diagrams which are well known to the mathematician and which he calls graphs.

A graph is a set of points in the plane called vertices whereby certain pairs of points are connected by lines called edges. The order of the graph is defined as the number of vertices. A graph is said to be connected if it consists of one piece only, otherwise disconnected.

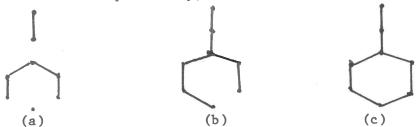


Fig 2 three graphs of order 8

- (a) disconnected graph
- (b) tree
- (c) graph with a loop.

The graphs of figure 1' are the carbon-skeletons of butane and isobutane.

The question arises: What properties do characterize a graph which is a possible carbon-skeleton for an alkane?

Clearly a necessary condition is that the <u>degree</u> of each vertex does not exceed 4, whereby the degree of a vertex is defined to be the number of edges incident at this vertex. Another necessary condition is that the number n of vertices (the order of the graph!) does exceed the number e of edges precisely by one:

$$(1)$$
 $n = e + 1$

In order to prove (1) let n_i be the number of vertices of degree i • (i = 1,2,3,4). Then obviously:

(2)
$$n_1 + n_2 + n_3 + n_4 = n$$

Moreover

(3)
$$n_1 + 2n_2 + 3n_3 + 4n_4 = 2e$$
.

In order to see the validity of (3) notice that if we count for each vertex the number of edges which are incident at this vertex and sum over all vertices then we count each edge twice.

Finally since the graph is derived from the structural formula of an alkane the equation

$$(4) \quad 3n_1 + 2n_2 + n_3 = 2n+2$$

must hold. Indeed each vertex of degree i corresponds to a C-atom which (in the structural formula) is linked to 4-i hydrogen atoms. Adding (3) and (4) we obtain

$$4(n_1 + n_2 + n_3 + n_4) = 2(e+n+1)$$

Since the left hand side equals 4n by (2) we obtain

$$2n = e + n + 1$$

which becomes (1) after cancelling n on both sides.

A connected graph with the property (1) is called a <u>tree</u>. A tree cannot contain any loop, since as soon as a loop is present in a connected graph the number of edges is at least as large as the number of vertices. Figure 2(c) illustrates this point; indeed for this graph e = n = 8.

Thus we arrive at the insight that a graph representing the carbon skeleton of an alkane must satisfy the conditions:

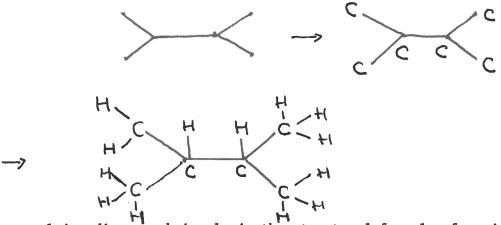
- (i) It is a tree.
- (ii) Every vertex has at most degree 4.

In fact these conditions are not only necessary but also sufficient. For suppose we are given a tree of order n satisfying condition (ii). We can construct the structural formula of an alkane from it by the following procedure: First affix to each of the n vertices the letter C; then plot for each vertex of valency i 4-i additional points with the letter H affixed to them and connect them to the vertex under consideration. The total number of new points you'll be adding in step 2 with the letter H affixed to them is:

$$3n_1 + 2n_2 + n_3 = 4(n_1 + n_2 + n_3 + n_4) - (n_1 + 2n_2 + 3n_3 + 4n_4)$$

= $4n - 2e = 4n - 2(n-1) = 2n+2$

where n again denotes the number of vertices of degree i in the given tree. This result makes it evident that the procedure just described produces from the given tree the structural formula of some alkane. Let us carry out the above procedure with the following tree of order 6



The resulting diagram obviously is the structural formula of an isomere of $^{C}_{614}$, i.e. hexane. Let us call a graph which enjoys properties (i) and (ii) above a $^{C-tree}$. Using this concept we can condense the insight attained so far into the sentence:

There is a one-to-one correspondence between the set of all isomeres of an alkane with a given number $\, n \,$ of C-atoms and the set of all C-trees of order $\, n \,$

Let us list all C-trees of order 6 and of order 7

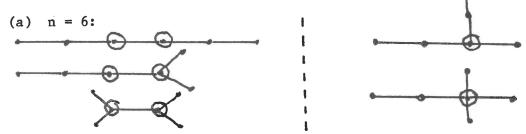
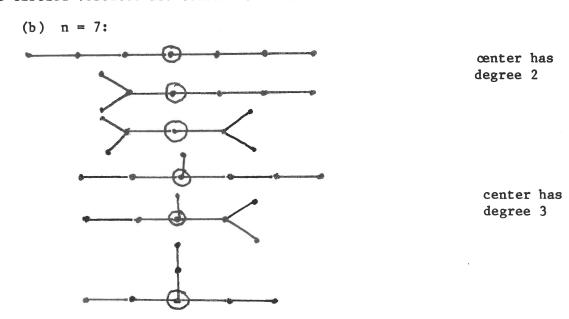
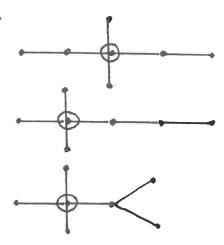


Fig. 3a. C-trees of order 6.

The circled vertices are central vertices





center has degree 4

Fig. 3b: C-trees of order 7
The unique central vertex is circled.

We see that there are 5 C-trees of order 6 and 9 C-trees of order 7. Hence there are 5 isomeres of hexane and 9 isomeres of heptane. Notice that in the plots of Fig 3 we circled those vertices which are <u>central</u>. What is the precise definition of a central vertex?

In order to arrive at such a definiton call the <u>eccentricity</u> ϵ of a vertex the maximal order of a branch incident at the vertex. The following examples of C-trees illustrate this concept:

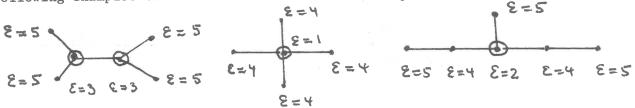


Fig 4. The eccentricity of a vertex.

Now a central vertex is simply defined as a vertex of minimal eccentricty.

Already in 1869 Camille Jordan²), proved that any tree of order n possesses either

(a) one central vertex of eccentricity $< \frac{n}{2}$

or

(b) two <u>adjacent</u> central vertices of eccentricity = $\frac{n}{2}$

Let us call a tree with property (a) <u>unicentered</u> and a tree with property (b) <u>bicentered</u>. Since the eccentricity of a vertex is necessarily an integer all trees of odd order must be unicentered. (Can you prove this directly?) This fact is illustrated by Figure 3b which shows that indeed all nine C-trees of order 7 are unicentered. In contrast the C-trees of order 6 (cf Fig 3a) consist of three bicentered trees and two unicentered trees.

Staring at the three bicentered C-trees of order 6 you may recognize that they are obtained by combining the two <u>rooted</u> trees of order 3



Fig 5: The two rooted C-trees of order 3

whereby a rooted C-tree is simply defined as a C-tree with one of its vertices of degree < 4 distinguished.

The following figure illustrates this observation

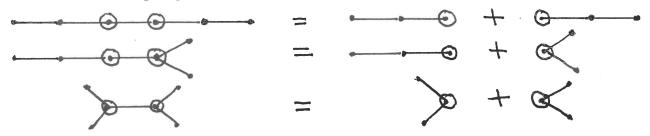


Fig 6: Every bicentered tree of order 6 is obtained by juxtaposition of two rooted bicentered trees of order 3.

This observation can be readily generalized: The bicentered C-trees of order n = 2s are obtained by combining two rooted C-trees of order s.

Given any natural numbers n let us introduce the following numbers:

r = # of rooted C-trees of order n

t' = # of unicentered C-trees of order n

t" = # of bicentered C-trees of order n

t = # of C-trees of order n = # of isomeres of the alkane

containing n C-atoms

Then clearly:

(5)
$$t_n = t'_n + t''_n$$

Moreover

(6)
$$t_n'' = \begin{cases} 0 & \text{if } n \text{ is odd} \\ 1/2 \cdot r_{n/2} & (r_{n/2} + 1) \text{ if } n \text{ is even.} \end{cases}$$

In order to understand the second half of formula (6) recall that the number of 2-combinations (with repetitions!) of r elements is precisely $\frac{1}{2}$ r (r+1). In case n = 6 the formula obviously gives the correct answer:

$$t_6'' = \frac{1}{2} r_3 (r_3 + 1) = \frac{1}{2} \cdot 2 \cdot 3 = 3$$

Formulae (5) and (6) show that we have solved our original problem completely if we have a solution to each of the following two problems:

- (1) For every natural number n find the number r of rooted C-trees of order n .
- (2) For every natural number $\, n \,$ find the number $\, t' \,$ of unicentered C-trees of order $\, n \,$

The solutions of the two problems as given by Polya take a similar form. They both can be expressed with the help of the polynomials $\frac{1}{2}$

(7)
$$p_k(x) = 1 + x + x^2 + 2x^3 + \dots + r_k x^k$$

whose coefficients are the numbers $(1,r_1,r_2,...r_k)$.

In fact a group theoretical analysis leads Polya to conclude that r_n is given as the coefficient of x^{n-1} in the polynomial

$$f_n(x) = \frac{1}{6} (p_{n-1}(x)^3 + 3p_{n-1}(x) p_{n-1}(x^2) + 2p_{n-1}(x^3))$$

This theorem has the character of a recursion formula, i.e. it allows us to compute r from the numbers r_1, r_2, \dots, r_{n-1} . As an example let us compute the number r_4 of rooted C-trees of order 4. r_4 is the coefficient of r_4 in the polynomial

(8)
$$f_4(x) = \frac{1}{6} (p_3(x)^3 + 3p_3(x)p_3(x^2) + 2p_3(x^3))$$

Now since $p_3(x) = 1+x+x^2+2x^3$ you can easily verify the correctness of the following table:

polynomial q	coefficient of	x ³ in q
P ₃ (x) ³	13	
$P_3(x)p_3(x^2)$	3	
p ₃ (x ³)	1	

Hence the coefficient of x^3 in $f_4(x)$ is:

$$r_4 = \frac{1}{6} (13+3\cdot 3+2\cdot 1) = 4$$

Indeed there are 4 rooted C-trees of order 4



Fig. 7: The rooted C-trees of order 4

obtained by distinguishing different C-atoms in the carbon skeleton of butane.

Similarly Polya proves that t' is given by the coefficient of x^{n-1} in the polynomial

$$g_n(x) = \frac{1}{24} (p_m(x)^4 + 6p_m(x)^2 p_m(x^2) + 3p_m(x^2)^2$$

+
$$8p_{m}(x) p_{m}(x^{3}) + 6p_{m}(x^{4})$$

where m is the largest integer smaller than $\frac{n}{2}$, i.e.

$$m := \begin{cases} \frac{n}{2} - 1 & \text{if } n \text{ is even} \\ \frac{n-1}{2} & \text{if } n \text{ is odd} \end{cases}$$

(Notice that by the theorem of Jordan mentioned above m is the largest possible eccentricity of the central vertex in a unicentered tree)

As an example let us compute the number t_8' of unicentered C-trees of order 8. t_8' is given as the coefficient of t_8' in the polynomial $g_8(x) = \frac{1}{24} (p_3(x)^4 + 6p_3(x)^2 p_3(x^2) + 3p_3(x^2)^2 + 8p_3(x)p_3(x^3) + 6p_3(x^4)).$

The following table gives the coefficients of x^7 in the various summands of g_{g} :

polynomial q

coefficient of x^7 in q

$p_3(x)^4$		100
$p_{3}(x)^{2}p_{3}(x^{2})$		14
$p_3(x^2)^2$		0
$p_3(x)p_3(x^3)$		1
p ₃ (x ⁴)		0

Thus the coefficient of
$$x^7$$
 in g is
$$t_8' = \frac{1}{24} (100+6.14+8) = 8$$

It follows that there are 8 unicentered C-trees of order 8 and $t_8'' = \frac{1}{2} r_4(r_4+1) = \frac{1}{2} \cdot 4 \cdot 5 = 10 \quad \text{bicentered trees of order 8.}$ Hence there are 10 + 8 = 18 isomeres of octane.

I highly recommend that you plot the 10 bicentered C-trees of order 8 by combining the four rooted C-trees of Fig. 7 in different ways and that you also sketch the 8 unicentered C-trees of order 8. You'll find that there are 5 unicentered C-trees whose center has degree 3 and 3 unicentered C-trees whose center has degree 4. In plotting these eighteen trees you'll get a vivid impression of the carbon skeletons of the different isomeres of octane.

One final remark: The number r of rooted C-trees of order n has a direct chemical significance. It gives you the number of isomeres of the alcohol (or any other monosubstitute for that matter) derived from an alkane. For instance the two rooted C-trees of order 3 (cf. Fig. 5) correspond to the alcohols

Propyl alcohol

isopropyl alcohol

A diluted form of the latter you can buy in the drug store under the name "Rubbing alcohol".

- George Polya: Kombinatorische Anzahlbestimmungen für Gruppen, Graphen & Chemische Verbindungen, Acta Mathematica 68, 145-254 (1937).
- 2. Camille Jordan: Sur les Assemblages de lignes, Journal für reine und angewandte Mathematik 70, 185-190 (1869).

EDITORIAL

[Views expressed in this section are those of the Editor and not necessarily (or even usually) those of the Department]

The crucial ingredient, required of the teacher, is patience. I found this in rather short supply when teaching my two young children to eat their porridge. Only the intervention of their mother prevents me from seizing the spoon myself. When it's all over (and all over everything), and they hold their bowls out with porridge-wreathed smiles and say - look clean bowl - I suppose it is worth it. But the mess is something fierce. At least it used to be.

We have less patience with adults than we have with children. There's no doubt who wields the spoon in my first-year Engineering class. In fact I use a shovel; you get more per scoop. You see, I'm on a tight schedule; the porridge has to be eaten by April. They still get it all over their faces, 'cause a shovel's pretty crude, and I often throw it before they get their mouths properly open, but a hellofalot gets down. At least I think it does.

One reason microcomputers can be such marvelous teaching tools is that they have infinite patience. The really creative mode is that in which the child is instructing the computer (rather than the reverse). The child can sit happily for hours without fear that the computer will pick up the spoon.

Of course the child can waste a lot of time sitting there too. At many points intervention is needed; real live teachers are still required. Thank goodness, this will always be so. Someone with a hand and a mind just like the child's must show her how to hold the spoon. We must intervene and we must stand aside. As usual, it's striking the balance that's so difficult.

Remainders in Base k

We were pleased to get a letter from Harry Occomore, Art's 41, in Bellevlle (15 Chelford Cres, K8N 4J8) with an intriguing divisibility result he calls the method of k factors. Let me quote part of his letter.

"Over 50 years ago I fell in love with Mathematics thanks to the late John Ross and James Davidson on the staff of Guelph Collegiate and Vocational Institute and I have never changed my mind on the subject. Now that I am retired (30 years as an Engineer with Bell Canada) I am enjoying myself delving into what my son (Electrical Engineering '70) calls useless side issues."

Harry's "useless side issue" is best illustrated with an example. Suppose you are given the number 6342510 written in base 7 and you need to find the remainder when it is divided by 5. Well, the answer turns out to be 2, and here's one way to find it.

Since 62 divided by 5 gives a remainder of 2, the answer's 2. The above calculation has 3 columns. The first contains the successive digits of the number, and the second contains the remainders when the successive powers of 7-5 are divided by 5. Thus, in the second column, the first entry is 2° , the second is 2° , the third 2° , the fourth 2° = 8 \equiv 3 (mod 5), and so forth. It turns out that the method works in general: if we are in base k and our divisor is d, the second column should always contain successive powers of k-d (mod d).

The question is, why does it work?

The Bureaucracy of Omnitopia - 2

[Tim Merrett (Queen's - Arts 64) is Associate Professor of Computer Science at McGill. He has contributed a number of times to the <u>Communicator</u>. This is a sequel to his March '81 article. He writes us that the theory of "mediate graphs" which derives from these little spoofs (?) is getting quite a bit of attention from the combinatorialists at McGill.]

Centuries after the founding of the Bureaucracy of Omnitopia, King Ruler was shrouded in myth and his rules were forgotten by all but scholars of dead languages:

Rule of Mediation. Access to any bureaucrat is mediated by another bureaucrat.

Rule of Buck-passing. Every bureaucrat mediates for some other bureaucrat.

The bureaucrats of Omnitopia came to call their mediators their "subordinates" and the bureaucrats they mediated for their "managers". They spent their days summarizing the reports from their subordinates and reporting on the summaries to their managers.

A young bureaucrat of an empirical turn of mind, Galley by name, made two discoveries that were to upset the Bureaucracy of Omnitopia forever. Galley was responsible for the machinery which printed the reports. Ond day he substituted for a report the sentence "There is an exception to every rule." (This sentence has been shown to be irreducible by Yodel, a famous mathematician who lived in a mountainous part of Omnitopia. It can therefore not be summarized.) He was able to observe that the same sentence was reported by each of 17 bureaucrats, of whom the last was the same as the first. The substitution and repetition were not noticed by the bureaucrats involved, but Galley had shown that cycles of managers (or subordinates) existed in Omnitopia.

Galley's second discovery was personally more calamitous, for those who rememberd and could expound King Ruler's rules in the original tongue were the guardians of culture and the arbiters of fortune for the bureaucrats of Omnitopia. He proved a violation of the Rules with himself as counterexample: Galley had no subordinates. He was forced to recant under pain of being replaced by a word processor. Galley had great integrity and was not afraid for himself, although he knew that removal from the Bureaucracy would doom him to a life of writing reports to himself in his own disjoint bureaucracy. But he also realized that if he were replaced by a word processor his proof would fail for want of a counterexample. So he recanted but, as he was reinstated in the print room, he murmered "it is true, nonetheless".

Exercise. Supply the details of Galley's proof.

DEPARTMENTAL NEWS

Bruce Kirby - was the winner last year of a Golden Apple, the excellence in teaching award of the Faculty of Applied Science.

Robin Giles - attended the first NAFIP (North American Fuzzy Information Processing Group) workshop in Utah in May, and presented a paper on Foundations of a Theory of Possibility.

Grace Orzech, Morris Orzech, Tony Geramita and Leslie Roberts
have all been invited to give hour talks on their research at the summer
meeting of the Canadian Math Society in Ottawa at the end of May. Also
Bill Higginson (Faculty of Education and Arts '65) is speaking in the
Educational Session on the Science and Education Study of the Science Council.
A quick scan of the program also revealed the name of Walter Whiteley
(Arts '66 - now at Champlain College) speaking in the Geometry Session.

<u>Rick Mollin</u> - accepted an invitation of Irving Reiner to speak in the algebra colloquium at University of Illinois (Urbana). Rick writes of this visit

"While I was there I was impressed not only by the size of the faculty (+150) but the quality of the work coming out of the Mathematics Dept there. Moreover the surrounding area is beautiful and full of activity. A cultural highpoint was a visit to the Kranert Art Museum where I picked up a copy of a painting by a Dutch artist Adrian Brouwer, who died at the age of 33. Other than that I have been able to find out nothing about this artist. I would be most interested in obtaining more information."

Rick has also been invited to speak at the Denisen conference in Columbus Ohio in June in honour of Hans Zassenhaus' 80th birthday. Right after this he heads for the finite simple groups conference in Montreal. Rick's energetic research work has paid off with an Associate Professorship at University of Calgary, effective September 1. Congratulations to Rick! Getting such a position these days is no mean feat.

Harold Still - has taken over from Tom Stroud as Chairman of Statistics
and

Dick Willmott - succeeds Norm Rice as Chairman of Undergraduate Studies.

PROBLEMS

Please send solutions to old problems and suggestions for new ones (with or without solutions) to the <u>Communicator</u>, Dept. of Mathematics and Statistics, Queen's University, Kingston, Ont. K7L 3N6.

Problem 7. NUMBER MATRICES WHICH ARE PRIME

By a number we mean a nonnegative integer: 0,1,2,3,... etc. By a number matrix we mean a 2×2 matrix $A = \begin{vmatrix} a & b \\ c & d \end{vmatrix}$ where entries a,b,c,d are numbers. We multiply number matrices as usual:

$$\begin{vmatrix} 4 & 2 \\ 3 & 1 \end{vmatrix} = \begin{vmatrix} 1 & 1 \\ 0 & 1 \end{vmatrix} \begin{vmatrix} 1 & 1 \\ 3 & 1 \end{vmatrix}$$

We first extend the notion of "prime" from the numbers to the number matrices.

Recall that a number $\, n \,$ is prime if it is not equal to a product of two numbers. Of course, we have to exclude two very simple products which always equal $\, n \,$. They are $\, n = n \cdot l \,$ and $\, n = l \cdot n \,$. Without this restriction, there wouldn't be any primes.

Observe that a number matrix A always equals each of

This leads us to make the following definition.

DEFINITION: A number matrix A is called prime if it cannot be written as the product of two number matrices except in the four simple ways given above.

The first question that arises is: "Have we excluded enough products". In other words, are <u>any</u> of the number matrices prime? [The answer is yes, of course].

PROBLEM: For each of the following number matrices, determine the values of the number n for which the matrix is prime:

$$\begin{vmatrix} n & 0 \\ 0 & 1 \end{vmatrix}$$
, $\begin{vmatrix} n & 0 \\ 0 & 2 \end{vmatrix}$, $\begin{vmatrix} 1 & n \\ 0 & 1 \end{vmatrix}$, $\begin{vmatrix} n & 1 \\ 1 & n \end{vmatrix}$, $\begin{vmatrix} n & 2 \\ 2 & n \end{vmatrix}$

David Gregory

SOLUTIONS TO PAST PROBLEMS

$$\frac{\text{Problem 5.}}{64} = \frac{1}{4}$$

How many quotients of two digit numbers are there for which a common digit can be cancelled?

Solution: Certain solutions of the problem are so easy to find as to be uninteresting and we will start by identifying them. For example,

$$\frac{20}{30} = \frac{2}{3}$$
 and $\frac{37}{37} = \frac{3}{3}$

are two such solutions. We can rule out these and similar solutions by insisting that at least one of the ones digits be non-zero and, as well, that the numerator and denominator be unequal. Let us agree to call all other solutions non-trivial.

The quotient of two two-digit numbers can be written in the form

 $\frac{10a+b}{10c+d}$, where a,b,c,d are integers with

 $1 \le a$, $c \le 9$ and $0 \le b$, $d \le 9$ (remember, $63 = 6 \times 10 + 3$). The cancellation of common digits can take one of three forms: the two tens digits are equal; the two ones digits are equal; or, the tens digit in the numerator and the ones digit in the denominator are equal. (There is a fourth form, in which the ones digit in the numerator and the tens digit in the denominator are equal, but this can be reduced to the third form by inverting the fraction). In the first case we require that

$$\frac{10a+b}{10c+d} = \frac{6}{d}$$
, $a = c$, and $b \neq d$, (1)

in the second case that

$$\frac{10a+b}{10c+d} = \frac{a}{c}$$
, $b = d$, $b = 0$ and $a = c$, (2)

and in the third case that

$$\frac{10a+b}{10c+d} = \frac{b}{c} \text{ and } a = d.$$
 (3)

(The inequalities in (1) and (2) come from ruling out the uninteresting solutions).

Let us start by considering the first case. The first two of the conditions listed in (1) yield (after a bit of algebra) the equation 10a(b-d)=0, and this equation has no solutions as $a\geq 1$ and as $b\neq d$. This means that the first case contains no solutions of the problem.

A similar argument will show that the second case also contains no solutions of the problem.

Now consider the third case. The two conditions listed in (3) together imply that

$$10ac = (9c+a)b$$
 (4)

As a and c are both non-zero this clearly implies that

$$b \neq 0 , \qquad (5)$$

and as 10 divides the left-hand side of (4) one of the following conditions must hold:

We will now proceed to analyze these three conditions.

If (6) holds then it is easy to see that the restrictions on a and c imply that a and c must be equal. But this means that we are back in the first case (i.e., that (1) holds) and so we again obtain no solutions of the problem.

If (7) holds then b=5 by (5) and 9c+a=2k for some integer k. Substituting b=5 and a=2k-9c into (4) and solving for k gives

$$k = \frac{9c^2}{2c-1}$$

This means that k=9 and a=9 if c=1, k=12 and a=6 if c=2, k=25 and a=5 if c=5, and all other allowed values of c=1 lead to non-integral k. This case therefore leads to the two non-trivial solutions

$$\frac{95}{19} = \frac{5}{1}$$
 and $\frac{65}{26} = \frac{5}{2}$.

All that remains now is to consider what happens if (8) holds. In this case we can write b=2s and 9c+a=5t for some s=1,2,3,4 and some integer t. Substituting b=2s and a=5t-9c into (4) and solving for t gives

$$t = \frac{9c^2}{5c-s}$$

If we now systematically replace c by $1, \dots, 9$ and s by 1, 2, 3, 4, select those pairs giving an integral t, and compute the corresponding values of a and b we get two more non-trivial solutions:

$$\frac{64}{16} = \frac{4}{1}$$
 and $\frac{98}{49} = \frac{8}{4}$.

The only solution which was submitted to this problem was by Mrs. Langlois, a mature student of John Waddington in the Grade 10 computer class of Thomas A. Blakelock High School in Oakville. She wrote a computer program to search for solutions (or, in her words, freaky fractions), and found them all. That's not a bad approach. It may well have taken her less time to do that than it took us to work out this algebraic solution. Well done Mrs. Langlois!

Problem 6:

Find integers m and n so that $3.14159 < \sqrt{m} - \sqrt{n} < \pi$.

Solution: (Karl Dilcher, Graduate student, Queen's). We can actually show a little more: There are integers m and N such that $3.14159 < \sqrt{m} - N < \pi$.

Proof: Let k be an integer, and put

$$n = (k-3)^2$$
, $m = k^2 + r$ (r an integer > 0).

Then $\sqrt{n} = k-3$, $\sqrt{m} = k\sqrt{1+\frac{r}{k}}$.

We may assume $r \leq k$; otherwise we would have $r \geq k+1$ and

$$\sqrt{m} - \sqrt{n} > \sqrt{k^2 + k + \frac{1}{4}} - (k-3) = k + \frac{1}{2} - (k-3) = 3.5$$

Now I claim
$$\sqrt{1+\frac{r}{k^2}} = 1 + \frac{1}{2} + \frac{r}{k^2} + R$$
, where $-\frac{1}{8k^2} < R < 0$.

This can be seen by using Taylor's formula, or simply by squaring:

$$(1+\frac{1}{2}\frac{r}{k^2})^2 = 1 + \frac{r}{k^2} + \frac{1}{4}\frac{r^2}{k^4} > 1 + \frac{r}{k^2}$$
 (since r>0)

$$(1 + \frac{1}{2} \frac{r}{k^2} - \frac{1}{8k^2})^2 = (1 + \frac{4r - 1}{8k^2})^2 = 1 + \frac{4r - 1}{4k^2} + \frac{(4r - 1)^2}{64k^4}$$

$$= 1 + \frac{r}{k^2} + \frac{(4r - 1)^2}{64k^4} - \frac{(4k)^2}{64k^4}$$

and since $r \leq k$, the sum of the last two terms is < 0 .

Now we have

$$\sqrt{m} - \sqrt{n} = k(1 + \frac{1}{2} \frac{r}{k^2} + R) - (k-3) = \frac{r}{2k} + kR + 3$$

That means, we have to find two integers r,k such that

$$0.14159 < \frac{r}{2k} + kR < 0.1415926 (<\pi)$$
.

We may choose
$$\frac{r}{2k} = 0.141592 = \frac{141592}{2(500000)}$$
, or better = $\frac{17699}{2(62500)}$

so take r = 17699, k = 62500. Now $-\frac{1}{8k} < kR < 0$, i.e. -.000002 < kR < 0,

i.e. with the above values of $\, r \,$ and $\, k \,$ we are within the required boundaries. Finally, we have

$$m = k^2 + r = 62500^2 + 17699 = 3906267699$$

and N = k - 3 = 62497.