The BIG SIGMAA News

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Business, Industry, and Government Special Interest Group of the Mathematical Association of America

Using Mathematical Models to Predict a Biological Response

adapted, with permission, from the University of Massachusetts Lowell Mathematics Department newsletter

Boehringer Ingelheim, a pharmaceutical company based in Ingelheim, Germany, had a problem: In medical research it is very important to know the biological responses to the compounds in drugs, but it is very expensive to determine this in trials because of the enormous number of possible combinations which must be tested. They needed a reliable method to determine the response to these compounds based solely on knowledge of their molecular properties (like size, shape, or elemental constitution). They had an extensive database of existing compounds and responses and wanted to use it to try to predict the response to new compounds.

So they approached Kaggle, a San Francisco based company that specializes in predictive modeling competitions. Companies, governments, and researchers present data sets and problems and scientists then compete to produce the best solutions. At the end of a competition, the host pays prize money in exchange for the intellectual property behind the winning models.

Jeremy Achin and Tom Degodoy

Thus was born the "Predicting a Biological Response" competition which, by the end of its three -month run (March 16 to June 15, 2012), had attracted close to 9,000 entries from more than 800 data scientists. Competitors were given 1,776 different variables, each representing a molecular descriptor pertaining to a characteristic of the molecule, and experimental data relating to actual biological responses. The aim was to predict which compounds hold the greatest promise so experimental efforts could be focused on them, while avoiding having to test others, only to

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Filling the Blank – My Time Helping SAT Preppers

by Greg Coxson

Several months ago, like too many engineers of my age, I found myself with a layoff notice and two weeks to start running . Having a family and a mortgage, I knew I needed a source of income while I looked for full-time work. One of my first stops was the local SAT prep office.

The timing was not the best, to put it mildly. The defense electronics industry, where I had worked for a number of years, was bracing for unprecedented rounds of cuts. When a colleague suggested I try tutoring, I was not excited about the idea. It did not take me long, however, to see the wisdom of his advice. If nothing else, I thought it might keep me busy and help keep my mind off of my situation.

There are a number of options for working as a tutor, and work at an SAT prep company is likely not the easiest. Another option is to sign up with a tutoring company and hang out an online shingle for professional one-on-one tutoring. It is possible to make quite a lot of money going this route; a colleague told me he was making nearly $1000 on a good Sunday tutoring time-pressed cadets at a military academy. While the money tends not to be as good at an SAT prep center, the hours are more reliable and all the materials you need (textbooks, folders of SAT

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Editor's note:

This is my first issue as editor of the BIG SIGMAA newsletter. In January I took over the duties of Vice Chair for Services of the BIG SIGMAA from Greg Coxon, who is now Vice Chair for Membership.

Thanks to Greg for contributed an interesting article for this issue. Thanks also to Collin Carbno for continuing to provide interesting artwork. If you would like to contribute an article, a poem, an puzzle, a limerick, or anything else to future issues of the newsletter, please let me know.

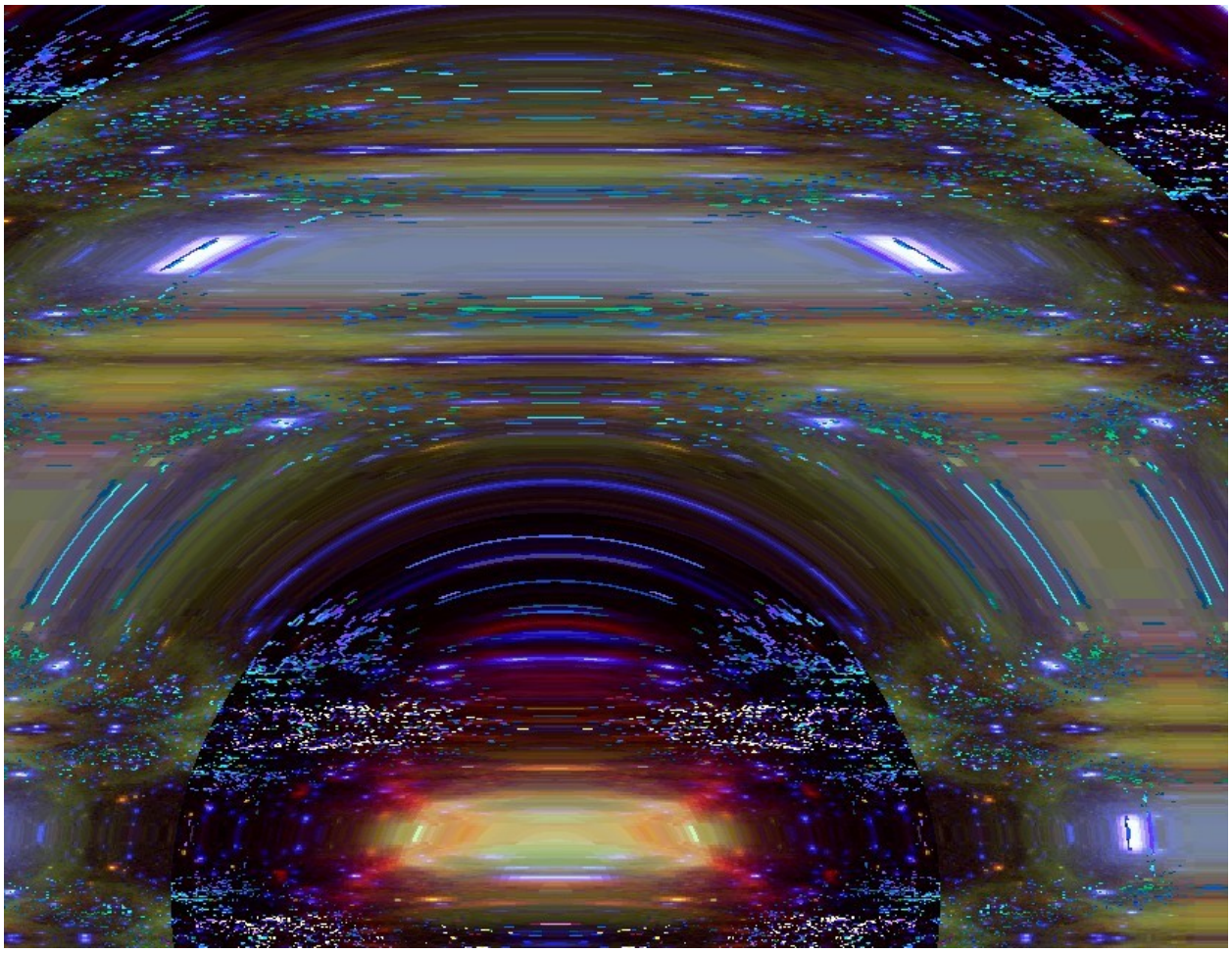
Jim Fife
Vice Chair for Services
BIG SIGMAA
jfife@ets.org.

Inside this issue:

Arithmetic

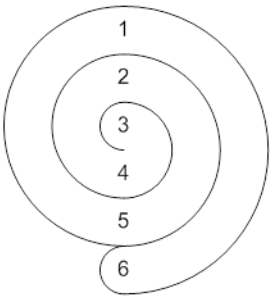
by Carl Sandburg

Arithmetic is where numbers fly like pigeons in and out of your head.
Arithmetic tells you how many you lose or win if you know how many you had before you lost or won.
Arithmetic is seven eleven all good children go to heaven – or five six bundle of sticks.
Arithmetic is numbers you squeeze from your head to your hand to your pencil to your paper till you get the answer.
Arithmetic is where the answer is right and everything is nice and you can look out of the window and see the blue sky – or the answer is wrong and you have to start all over and try again and see how it comes out this time.
If you take a number and double it and double it again and then double it a few more times, the number gets bigger and bigger and goes higher and higher and only arithmetic can tell you what the number is when you decide to quit doubling.
Arithmetic is where you have to multiply – and you carry the multiplication table in your head and hope you won't lose it.
If you have two animal crackers, one good and one bad, and you eat one and a striped zebra with streaks all over him eats the other, how many animal crackers will you have if somebody offers you five six seven and you say No no no and you say Nay nay nay and you say Nix nix nix?
If you ask your mother for one fried egg for breakfast and she gives you two fried eggs and you eat both of them, who is better in arithmetic, you or your mother?



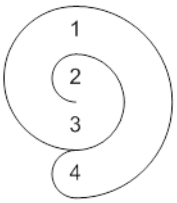
Energizer Field by Collin Carbno

Sestinas



At the 2009 Joint Meetings, the last time the meetings were in Washington, Michael Saclolo of St. Edwards University gave a talk in the Arts SIGMAA session about the mathematics behind a form of poetry called a *sestina*. A sestina is a poem consisting of six 6-line stanzas, followed by one 3-line stanza. There is no rhyme scheme; instead the ending words of the lines in each stanza are a particular permutation of the ending words of the lines in the previous stanza; this permutation can be obtained from the spiral figure shown on the right. If the numbers 123456 represent the ending words of the first stanza, then the order in which these words appear in the second stanza can be read from the spiral by starting at the bottom, with 6, and following the spiral; the order is 615243. The word at the end of line 6 in the first stanza becomes the word at the end of the first line of the second stanza, the word at the end of line 1 in the first stanza becomes the word at the end of the second line in the second stanza, and so on. This permutation can be represented schematically as

6→1 1→2 5→3 2→4 4→5 3→6



This is the cycle (1 2 4 5 3 6). The permutation must be a six-cycle so that each ending word is in a different line in each stanza. The form was developed by the French troubadour Arnout Daniel de Riberac in the twelfth century.

If the number of lines in each stanza equals some number $n \neq 6$, the permutation need not be an n-cycle. For example, if $n = 4$ we see from the spiral figure on the right that the order is 4132, which is the permutation (1 2 4) (3). The word ending the third line in never permuted; it ends the third line of each stanza.

There is a necessary condition that the permutation be an n-cycle: If the permutation is an n-cycle, then $2n + 1$ is prime. The condition is not sufficient, however. For example, if $n = 8$, the permutation is the product of two 4-cycles: (1 2 4 8)(3 6 5 7), and hence the pattern of ending words would repeat after four lines.

More details can be found in Dr. Saclolo's paper "How a Medieval Troubadour Became a Mathematical Figure", *Notices of the AMS* **58** (5): 682-7.

Here is a famous sestina by Rudyard Kipling, in which he delivers the twelfth-century French form in a Cockney accent.

Sestina of the Tramp-Royal

SPEAKIN' in general, I 'ave tried 'em all—
The 'appy roads that take you o'er the world.
Speakin' in general, I 'ave found them good
For such as cannot use one bed too long,
But must get 'ence, the same as I 'ave done,
An' go observin' matters till they die.

What do it matter where or 'ow we die,
So long as we've our 'ealth to watch it all —
The different ways that different things are done,
An' men an' women lovin' in this world —
Takin' our chances as they come along,
An' when they ain't, pretendin' they are good?

In cash or credit—no, it aren't no good;
You 'ave to 'ave the 'abit or you'd die,
Unless you lived your life but one day long,
Nor didn't prophesy nor fret at all,
But drew your tucker some'ow from the world,
An' never bothered what you might ha' done.

But, Gawd, what things are they I 'aven't done?
I've turned my 'and to most, an' turned it good,
In various situations round the world—
For 'im that doth not work must surely die;
But that's no reason man should labour all
'Is life on one same shift—life's none so long.

Therefore, from job to job I've moved along.
Pay couldn't 'old me when my time was done,
For something in my 'ead upset me all,
Till I 'ad dropped whatever 'twas for good,
An', out at sea, be'eld the dock-lights die,
An' met my mate—the wind that tramps the world!

It's like a book, I think, this bloomin' world,
Which you can read and care for just so long,
But presently you feel that you will die
Unless you get the page you're readin' done,
An' turn another—likely not so good;
But what you're after is to turn 'em all.

Gawd bless this world! Whatever she 'ath done—
Excep' when awful long—I've found it good.
So write, before I die, "'E liked it all!"

Filling the Blank – My Time Helping SAT Preppers

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and other tests, with answer keys) are close at hand.

At the place I chose, it is necessary to take SAT tests to show some mastery of the material. That was actually kind of fun, and I came home joking "I've still got it" (my kids told their friends I did the SAT "without a calculator!"). In addition, there are mandatory online training courses on how to tutor. Having worked as a teaching assistant in Mathematics for several years, I found this a bit of an annoyance at first. I quickly cast off that feeling; the training was serious and taught me new skills.

I worked two or three days a week, in two or three consecutive two-hour sessions. In each session, I would have from one to three students. Because I was more specialized than other tutors, I tended to get mostly Mathematics assignments, everything from Trigonometry to Calculus.; I even helped one cute earnest second grader through exercises like "measure your textbook". Each session tended to involve both weak and strong students. I was trained to spend more time with the weaker students, allowing the stronger students more independence to work on exercises that I would return to check at intervals. Ultimately, I also got assignments to work with a competition-Math student; those sessions tended to be one-on-one work since the problems required more focus.

I came to respect my peers on the tutoring staff. Most of the tutors are young, either about to start graduate school or in some stage of PhD programs. Some are parents who needed the extra income. Some are retired teachers. One had left a PhD program in Chemistry to do day trading, before losing millions in the stock market crash. What impressed me the most were the tutors who could work in several topics, and provide timely help using an array of tutoring skills. It takes a special person to be able to take on AP Calculus, Honors Spanish, American Government, and Chemistry, all in one evening. At times it seemed I had found a hidden world of Renaissance scholars.

I learned a lot from my students as well. The environment is more competitive than when I was in high school. Many of these students have a keen idea of what college they can hope to gain entry to, as early as sophomore year. I got to know their dreams and plans. One student wants to design high-performance cars for the general market, another wants to be an international lawyer focused on children's issues, another is working on adding 2 mph to his fastball. The experience opened my eyes to the level of competition my kids face. It also gave me an inside look at the relative strengths of almost every private or public high school within about 20 miles of the center.

Eventually my tutoring tailed off. I started teaching a Calculus I course at a local community college. After six months, I began full-time employment in my field. Still, I value the time I spent in the world of SAT prep.

Joint Mathematics Meetings—San Diego Meeting

The 2013 version of the Joint Mathematics Meetings met in San Diego in January. Over 6,600 people attended the conference, enjoying mathematics lectures, exhibits, and artwork. It was also an opportunity to see old friends and make new ones. Usually, when the Joint Meetings are in San Diego, it's also an opportunity for those of us who live in the colder parts of the country to experience some warmth and sunshine in January. But this year the weatherperson seems not to have received the memo, as the weather was cool and quite windy.

But the conference was amazing, nonetheless, with many fine sessions. In particular, the BIG SIGMAA sponsored a well-attended talk by Mario Livio, the author of the book *Is God a Mathematician?* Dr. Livio's talk, along with the shorter talks in the BIG SIGMAA paper session, are described in Carla Martin's article in the February/March issue of FOCUS; you can download the issue from the MAA's website .

Next year's Joint Meetings in Baltimore is shaping up to be just as interesting. Watch the MAA website and the BIG SIGMAA website (sigmaa.maa.org/big) for details as they become available. We hope to see all of you in Baltimore.

Limerick

A mathematician I know
Can count to a million or so.
But should he regress,
He'll then coalesce
And back to the mean he will go.

Predicting a Biological Response

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have them ultimately prove ineffective.

In one of the first times "gamification" has provided such a practical contribution to drug development, and despite the fact that the competitors had no particular knowledge of the pharmaceutical industry, results of the competition revealed the best models to be more than 25% more effective than those currently in use. The winning model was submitted by a team of three data scientists, Jeremy Achin and Tom Dogedoy (both alumni of the University of Massachusetts Lowell) and Sergey Yurgenson, a Research Associate in Neurobiology at Harvard Medical School. The winning team won a $10,000 prize.

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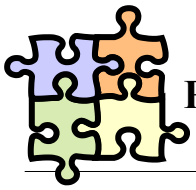
Business • Industry • Government
Special Interest Group of the MAA

from the MAA Website:

BIG SIGMAA serves as a unifying link between business, industry and government mathematicians, academic mathematicians, and mathematics students. The SIGMAA provides resources and a forum for MAA members who share an interest in mathematics used in business, industry and government, aids in professional development, helps build partnerships between industry and academics, and increases awareness of opportunities for mathematicians in business, industry and government.



Puzzle Corner: Chocolate Pudding

This is an old puzzle, but it's still interesting. I was reminded of it when a colleague sent it to me a couple of years ago.

A mathematician was attending a party at the host's house and had a conversation with the host:

Mathematician: How many children do you have?
Host: I have three daughters.
Mathematician: What are their ages?
Host: The product of their ages equals 72.
Mathematician: That's not enough information for me to determine their ages.
Host: The sum of their ages equals my house number.
Mathematician: I still don't have enough information to determine their ages.
Host: My oldest daughter likes chocolate pudding.
Mathematician: Ah, in that case, the ages of your daughters are ….

What are the ages of the host's daughters? (Assume the ages of the daughters are whole numbers.)

Of course, knowing only that the product of the ages is 72 and the sum is the unknown house number is not sufficient to determine the ages. But, although we don't know the host's house number, the mathematician presumably does (after all, he's at the host's house) and the mathematician cannot determine the ages, either. Therefore there must be at least two sets of three integers whose product is 72 and whose sum is the host's house number.

By looking at all possible sets of three integers whose product is 72, it is easy to see that 14 is the only integer that can be expressed in two ways as the sum of three integers whose product is 72 ($14 = 6 + 6 + 2$ and $14 = 8 + 3 + 3$). Thus the ages of the host's daughters are either 6, 6, and 2 or 8, 3, and 3.

This is where the clue about chocolate pudding comes in. The significance of that clue is that the host *has* an oldest daughter; in other words, the oldest two daughters are not twins. Therefore the ages of the daughters are 8, 3, and 3.