What Is Experimental Mathematics?

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Abstract: It is not what you think.

Why Am I Giving This Talk?

Thank you all for coming! I really appreciate you showing up. As for the many colleagues and grad students who did *not* show up, thanks also! Now I won't feel obligated to come to your talks, or in the case of grad students, agree to be on your oral committee, or write you a letter of recommendation.

One of the reasons I agreed to give this colloquium talk was to find out who are the good guys and who are the bad guys in this department. Of course, those who are here (and won't leave early) are the good guys, and their complement are the bad guys. I believe that one should show up to as many colloquium talks as possible, even if , and in fact, especially if, they are far removed from one's narrow specialty. It is like going to Church on Sunday, to Synagogue on Saturday, or Mosque on Friday. My student Eric Rowland will soon take a picture of the audience and this way I'll know who is here. I promise to always come to any talk that any of *you* will give, or sponsor. I also promise *not* to come to any talk given or sponsored by faculty or grad students who are not here right now, unless it is really really interesting.

So that was the first reason for giving this talk. The second reason is to illustrate **by example**, how to give a perfect colloquium talk, accessible to everyone. The third reason is to illustrate the **Zeilberger methodology** of teaching Freshman Calculus. The main ingredients of my method are the **handout** and the **"quiz"**. In each and every one of my classes, I give out a handout, explaining in excruciating detail how to do the homework problems from the covered section. Then, in the last five minutes, everyone has to attempt a "quiz" that does not count towards the grade, except that it is used to check attendance (attendance is strictly mandatory in my classes). I ask my students to write their name and E-mail address, and for those who didn't get it perfectly right, I write them an E-mail explaining what they did wrong. I know that you are not freshmen, but still, just to illustrate my method, I will give out a "quiz" at the end of my talk and will write you E-mail on Monday in case you didn't get it right.

Last, but not least, the fourth reason for giving this talk is to tell you about experimental mathematics the way I and my students practice it. It is not the conventional way!

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The Experimental Math Group at Rutgers

Speaking of my students, together with Hill Assistant Professor Drew Sills, and myself, they comprise the Experimental Mathematics Group here at Rutgers. We have a weekly seminar, that meets at Hill 705 every Thursday between 5:00pm and 5:50pm, that has (usually) exciting talks. You are all welcome to come as often as you wish.

Let me describe very briefly what they are up to. For more details, see their websites.

Drew Sills is one of the greatest experts in the world in RogersRamanujanology and developed a great package, `RRtools`, for exploring (and proving!) fascinating results in that theory. In collaboration with me, we taught the computer how to automatically discover and *prove* far-reaching extensions of the celebrated Dyson Constant Term Identity (first proved by physics Nobelist Ken Wilson). **Moa Apagodu** does beautiful extensions and applications of WZ theory. **Lara Pudwell** and my recently graduated student **Vince Vatter** teach computers how to enumerate permutations much more efficiently (and rigorously!) then any human can do. **Eric Rowland** does, among other things, Cellular Automata, in the style of Stephen Wolfram. **Thotsaporn Thanatipanonda** (a.k.a. "Aek") teaches computers how to play *Chess* but, unlike Deep Blue and Deep Junior, not on an 8×8 board (this is not math!) but on an $m \times n$ board. He was able to find better winning strategies, even for $m = n = 8$, then those suggested by former world champion Jose Capablanca in his classic book. For now, of course, he does simple endgames, but I am sure that he will be able to do increasingly more complicated positions. I should also mention **Arvind Ayyer**, whose work is not exactly experimental mathematics, but it is very interesting nevertheless, applying combinatorial identities to string theory.

Finally, What is Experimental Math?

Let me try and explain to you, by example, what is experimental math. It is really an *attitude* and *way of thinking*, or rather *not thinking*. Mathematicians traditionally love to solve problems by **thinking**. Myself, I hate to think. I love to **meta-think**, try to do things, whenever possible, by **brute force**, and of course, let the computer do the hard work.

I just came back from a conference in Florida, and one of the other plenary speakers, the famous Michigan number theorist **Hugh Montgomery**, who is also an avid problem-solver (and hence a closet combinatorialist) told me about a cute problem that he proposed for the Putnam exam- on whose committee he is currently serving- and that was rejected by the other members of the committee for being "too hard". He wrote it down on a napkin[2] [the napkin is shown to the

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[2] It was during the reception on March 6, 2006, of the 37th International Southeastern Conference on Combinatorics, Graph Theory and Computing held at Florida Atlantic University. On the same napkin, Hugh Montgomery scribbled the following challenging problem. "Let I and J be intervals on the real line, and let q and r be integers, $q \geq 1$. If $|I| \cdot |J| < q$ then $\{n \in I : rn \in J(mod\ q)\}$ is a segment of an arithmetical progression." This interesting problem was mailed to Montgomery, in the mid seventies, from a cabin in Montana, by the Michiganer alumnus T.J. Kaczynski.

audience], and here it is:

Hugh Montgomery's Rejected Putnam Proposal

Show that there exists a polynomial $P \in R[x,y]$, $P \neq 0$, such that $P(F_n, F_{n+1}) = 0$ for every n, where F_n are the Fibonacci numbers defined by $F_0 = 0, F_1 = 1$ and $F_n = F_{n-1} + F_{n-2}$ for $n \geq 2$.

The Experimental Math Approach

Go to Maple and type

```
with(combinat):  P:=(d,x,y)->add(add(a[i,j]*x**i*y**j,i=0..d-j),j=0..d);

V:=d->{seq(seq(a[i,j],i=0..d-j),j=0..d)};

E:=d->{seq(P(d,fibonacci(n),fibonacci(n+1)),n=1..nops(V(d))+5) }:

Q:=(d,x,y)->subs(solve(E(d),V(d)),P(d,x,y));
```

Now type `Q(1,x,y);` and get 0, which is correct, but does not count, since Hugh Montgomery insisted on a *non-zero* polynomial. Then we try, in turn, `Q(2,x,y);` and `Q(3,x,y);` and still get 0. But type `Q(4,x,y);`, *et voilà*, Maple returns the answer

$$(x^2 + xy - y^2 - 1)(x^2 + xy - y^2 + 1) \quad ,$$

implying the *Fibonacci identity* relating two consecutive Fibonacci numbers

$$(F_n^2 + F_n F_{n+1} - F_{n+1}^2 - 1)(F_n^2 + F_n F_{n+1} - F_{n+1}^2 + 1) = 0 \quad .$$

Now most of you would say, 'that's very nice, but it is only a conjecture, we still need humans to prove it for *all* n'. Nonsense! Once discovered, any polynomial identity (and many other types!) involving Fibonacci numbers, like the one above, is routinely and automatically provable by computer. Why? (hint: Binet's formula).

Now to do this, it took me one minute to type the Maple code (since I am a slow typist), and took the computer less than a second to discover (and prove) the above polynomial identity. In fact, in this case (and in many other cases), there is no need for a proof, using, say, Binet's formula alluded to in the paragraph above. By general linear algebra nonsense it is easy to show that if the identity is true for sufficiently many special cases, it is true for every n, and since *E(d)* was defined with a few equations to spare, everything is watertight.

I am not sure how Hugh Montgomery solved this problem, but I am sure that it took him more than a minute.

For the sake of the Maple illiterate, let me explain what the code means. $P(d,x,y)$ defines a generic polynomial of x and y of degree d, with *undetermined coefficients.*

$$P(d,x,y) := \sum_{j=0}^{d} \sum_{i=0}^{d-j} a_{i,j} x^i y^j \quad ,$$

while $V(d)$ is the set of coefficients:

$$V(d) := \{a_{i,j} \quad | \quad i \geq 0, j \geq 0, i+j \leq d\} \quad .$$

$E(d)$ is the set of equations

$$E(d) := \{P(F_n, F_{n+1}) = 0 \quad | \quad 1 \leq n \leq |V(d)| + 5\} \quad .$$

Finally, `solve(E(d),V(d))` solves the system of $|V(d)|+5$ equations and $|V(d)|$ unknowns, and $Q(d,x,y)$ substitutes the general solution into $P(d,x,y)$.

Experimental Mathematics through the ages

Until relatively recently, about 2500 years ago, *all* of mathematics was experimental. The sages of ancient Egypt, Sumer, Babylon, India and China had a very advanced empirical science. Then came Euclid and his cronies (who had an axe to grind with Zeno and other skeptics) and invented the axiomatic method, and turned mathematics into a *deductive* science, at least officially. Of course, all the great mathematicians (and also the not so greats) *implicitly* did experiments (until sixty years ago, with pencil and paper [or finger and sand, but watch out for Roman soldiers]), but most of them covered their traces and didn't tell anyone.

Leonhard Euler: Experimental Mathematician

One of the few giants who did not make any bones about empirical discoveries was the great Euler. Possibly because of his friend Goldbach, he was interested in a characterization of prime numbers. He may have also had in mind the problem of proving that there are infinitely many perfect numbers and that there are no odd perfect numbers. Now a good way to characterize both *prime* and *perfect* numbers is via the *sum of divisors* function $\sigma(n)$

$$\sigma(n) = \sum_{d|n} d \quad .$$

For example $\sigma(6) = 1+2+3+6 = 12$. Now p is a prime iff $\sigma(p) = p+1$ and n is perfect iff $\sigma(n) = 2n$. So if you know everything about $\sigma(n)$ you would be able to do Goldbach, Twins, and Perfect.

The first item on the agenda is to *compute* the first thousand, or so, values of $\sigma(n)$. Since factoring is hard, it would be nice if one could only use addition and subtraction, and be able to use previously computed values of σ. So Euler tried to find some kind of recurrence. Here is how he reasoned.

First he used what Herb Wilf calls *generatingfunctionology.* Obviously, if $d(n)$ is the *number of divisors* of n, then

$$\sum_{n=0}^{\infty} d(n)x^n = \sum_{i=1}^{\infty} \frac{x^i}{1-x^i} \quad ,$$

since the $x^i/(1-x^i)$ contributes one term to each of the multiples of i. Now for the *sum* of divisors, one has similarly

$$\sum_{n=0}^{\infty} \sigma(n)x^n = \sum_{i=1}^{\infty} \frac{ix^i}{1-x^i} \quad .$$

But the right side is essentially the logarithmic derivative of $(1-x^i)$, so we have

$$\sum_{n=0}^{\infty} \sigma(n)x^n = -x\sum_{i=1}^{\infty}[\log(1-x^i)]' = -x\left(\log\left[\prod_{i=1}^{\infty}(1-x^i)\right]\right)' = -x\frac{\Pi'}{\Pi} \quad ,$$

where

$$\Pi = \prod_{i=1}^{\infty}(1-x^i) \quad .$$

Now, just with pencil and paper, Euler expanded the first forty or whatever terms of this infinite product to get

$$\Pi = 1 - x - x^2 + x^5 + x^7 - x^{12} - x^{15} + x^{22} + x^{26} - x^{35} - x^{40} + etc.,$$

[Euler used 'etc.' instead of $\ldots$], and he immediately recognized the exponents as **pentagonal numbers**, and made the

Conjecture:

$$\prod_{i=1}^{\infty}(1-x^i) = 1 + \sum_{j=1}^{\infty}(-1)^j[x^{j(3j-1)/2} + x^{j(3j+1)/2}] \quad ,$$

but couldn't find a **demonstration**. He said that he had a *preuve*, by which he meant an empirical proof, but lacked a *demonstration*, meaning a formal proof. Nevertheless, being a true experimental mathematician, it did not stop him from drawing important consequences, and he postponed the task of finding a complete proof to when he'll get around to it.

Now, he multiplied both sides of

$$\sum_{n=0}^{\infty} \sigma(n)x^n = -x\frac{\Pi'}{\Pi} \quad ,$$

by Π, getting

$$\Pi\sum_{n=0}^{\infty} \sigma(n)x^n = -x\Pi' \quad ,$$

and assuming his conjecture for now, and comparing coefficients of x^n on both sides he derived a recurrence for $\sigma(n)$:

$$\sigma(n) = \sum_{j=1}^{[\sqrt{2n/3}]} (-1)^{j-1}[\sigma(n-j(3j-1)/2) + \sigma(n-j(3j+1)/2)] \quad ,$$

if n is not a pentagonal number, and if n is a pentagonal number $n = k(3k \pm 1)/2$, then

$$\sigma(n) = \sum_{j=1}^{[\sqrt{2n/3}]} (-1)^{j-1}[\sigma(n - j(3j-1)/2) + \sigma(n - j(3j+1)/2)] + (-1)^{k+1}n \quad ,$$

that enabled Euler to compile a table of $\sigma(n)$ for $n \leq N$ in time $O(N^{3/2})$.

Only twenty five years later, when he was more then seventy years old, did he find a formal proof. Of course, he did lots of other things in between, but we should learn from him not to get hung up on one step.

Carl Friedrich Gauss: Experimental Mathematician

Also the great Guass was an excellent experimental mathematician, although you wouldn't know it from his *published* work. But his fascinating diary contains lots of experimentations. For example, consulting tables of prime numbers, he guessed the **Prime Number Theorem** that $\pi(n)$, the number of primes less than n is asymptotically $n/\ln n$:

$$\pi(n) \sim \frac{n}{\ln n} \quad .$$

Srinivasa Ramanujan: The Greatest Experimental Mathematician

Srinivasa Ramanujan had an amazing intuition on what is interesting and correct and he conjectured lots and lots of results that took many mathematician-hours to prove formally, and some of his discoveries are still being proved today by Bruce Berndt, George Andrews, and their disciples. Some of his results he proved himself, after G.H. Hardy tried to teach him about 'proof', but I am sure that he was only trying to be nice to Hardy, and he had no doubt that his discoveries were correct, even without a formal proof.

One of his most famous results, that

$$p(5k+4) \equiv 0 \,(mod \;\, 5) \quad ,$$

where $p(n)$ is the *number of integer partitions* of n was discovered when he looked at the table of this sequence computed by Percy MacMahon using the recurrence

$$p(n) = \sum_{j=1}^{[\sqrt{2n/3}]} (-1)^{j-1}[p(n - j(3j-1)/2) + p(n - j(3j+1)/2)] \quad ,$$

that is very similar, but slightly simpler then Euler's recurrence above for $\sigma(n)$. It also follows from Euler's Pentagonal Number Theorem (even simpler, there is no need to take the logarithmic derivative), as was first observed by Euler.

The Computer Age

Many parts of modern math, for example *fractals* and *chaos* wouldn't be possible without experimentation done on the computer. This is obvious. However, I know of quite a few important theorems in very pure math that were discovered by computer experimentation, but the ungrateful human author never even acknowledged this fact!

Mitchell Feigenbaum

Playing with a programmable calculator that his parents bought him as a graduation present, a young postdoc at Los Alamos, in the early seventies, was iterating the mapping

$$x \to \lambda x(1-x) \quad , \quad (0 < x < 1)$$

for various values of λ, and noticed that for small values of λ it tends to just one limiting value (regardless of the starting number), then suddenly, in the long run, it alternates between two limiting values, then 4, then 8, etc, until chaos rules completely. Not only that, calling the cutoffs values of λ, λ_1, λ_2, λ_3, etc., Feigenbaum noticed that

$$\lim_{n\to\infty} \frac{\lambda_{n+1}-\lambda_n}{\lambda_n-\lambda_{n-1}} = 4.669\ldots \quad ,$$

the *now* famous Feigenbaum constant. The rest is history.

Bailey-Borwein-Plouffe

There are lots of formulas for π, some converge extremely slowly, like Leibnitz's

$$\pi = 4\sum_{n=0}^{\infty} \frac{(-1)^n}{2n+1} \quad ,$$

and some very fast. But the following beautiful formula,

$$\pi = \sum_{n=0}^{\infty} \left(\frac{4}{8n+1} - \frac{2}{8n+4} - \frac{1}{8n+5} - \frac{1}{8n+6} \right) \frac{1}{16^n} \quad ,$$

due to David Bailey, Peter Borwein, and Simon Plouffe is special, since it enables one to compute the zillionth and first binary digit of π without having to first compute the previous zillion digits. Once known, its proof is an easy calculus exercise, but *discovering* it, using the methodology of *experimental mathematics*, was a major tour-de-force.

If you want to know more about 'mainstream' experimental mathematics read the wonderful two-volume set on this subject written by David Bailey and Jon Borwein (v.1) and Bailey, Borwein and Roland Girgensohn (v.2).

Zeilberger-style Experimental Mathematics

Traditionally there was a **dichotomy** between the **context of discovery**, that nowadays is mostly done by computers, and the **context of verification** that is still mostly carried out by humans. In my style of experimental math, the computer does *everything*, the *guessing* and the (rigorous!) *proving*, if possible completely seamlessly without any human intervention. Feel free to browse my website for many examples.

Handout Time

As I promised, I will now hand out a **handout**, that illustrates the methodology in terms of a very simple example, that of the classical **gambler's ruin**.

Dr. Z's March 10 Colloquium Handout

Problem Type: A function is given by some rule. First conjecture, and then rigorously prove, an explicit formula for it.

Example Problem: Let $f_L(n)$ be the expected life of a gambler in a fair casino, who currently has n dollars and loses or wins a dollar with probability $1/2$, and has to quit when he is ruined, or when he has L dollars. Find an explicit formula for $f_L(n)$ as a function of n and L.

Steps

1. Using human (or computer) ingenuity, set up an algorithm for computing the function numerically for "small" values of the arguments.

Example

1. For a fixed L, the $n+1$ quantities $f_L(n)$ $(n = 0 \dots L)$ are completely characterized by the system of $n+1$ linear equations with $n+1$ unknowns

$$f_L(n) = \frac{1}{2} f_L(n-1) + \frac{1}{2} f_L(n+1) + 1 \quad , \quad (1 \le n \le L-1)$$

$$f_0(0) = 0 \quad , \quad f_L(L) = L \quad .$$

2. Using a linear solver, crank out enough data.

2.

$$f_3(0)=0, f_3(1)=2, f_3(2)=2, f_3(3)=0 \quad ,$$

$$f_4(0)=0, f_4(1)=3, f_4(2)=4, f_4(3)=3, f_4(4)=0 \quad ,$$

$$f_5(0)=0, f_5(1)=4, f_5(2)=6, f_5(3)=6, f_5(4)=4, f_5(5)=0 \quad .$$

3. Conjecture an *ansatz* and use *undetermined coefficients* to find it (if possible).

3. Setting $f_L(n)=an^2+bn+c$ and solving for a,b,c (for each specific L) we get

$$f_3(n)=n(3-n) \quad f_4(n)=n(4-n) \quad f_5(n)=n(5-n)$$

$$f_6(n)=n(6-n) \quad , \quad f_7(n)=n(7-n) \quad .$$

4. Using the same methodology conjecture an expression in L for $f_L(n)$, then prove it *rigorously* by using the *defining algorithm*, but now **symbolically**.

4.

$$f_L(n)=n(L-n) \quad .$$

Now let's prove it! Let's denote $g_L(n):=n(L-n)$. We have

$$g_L(n)-\frac{1}{2}g_L(n-1)-\frac{1}{2}g_L(n+1)-1=$$

$$L(n-L)-\frac{1}{2}(n-1)(L-(n-1))-\frac{1}{2}(n+1)(L-(n+1))-1=0 \quad .$$

Also $g_L(0)=0\cdot(L-0)=0$ and $g_L(L)=L(L-L)=0$. So we have a **rigorous** proof that $f_L(n)=g_L(n)$ for *every* n and L.

Quiz Time

As I promised you, now you have a chance to test your understanding. Here is the "quiz". I am sure that most of you will get it right, but in case you don't, I'll be writing you an E-mail on Monday, explaining your errors.

"QUIZ" for March 10, 2006, Dr. Z.'s Colloquium talk

NAME: (print!) ______________________________

E-MAIL ADDRESS: (print!) ______________________________

1. Conjecture and prove an explicit expression for

$$a(n) := \sum_{i=1}^{n} i$$

using the methodology of **experimental mathematics** (no credit for other methods!) .

Hint: $a(n)$ is characterized by $a(n) - a(n-1) = n$ and $a(0) = 0$.

APPENDIX

Who handed in the quiz?

Arvind Ayyer, Dick Bumby, Greg Cherlin, "Deep Purple", Sue Geller [visiting from Texas A&M], Zheng-Chao Han, Jim Lepowsky, Laurie Moore, Roger Nussbaum, Amit Priyadarshi, Lara Pudwell, Eric Rowland, Drew Sills, Thotsaporn Thanatipanonda ("Aek"), Roderich Tumulka [visiting from Tuebingen], Jerrold Tunnel, Liming Wang, Chuck Weibel, Robert Wilson.

You all did a great job! Thanks.

Answer to the Quiz

By direct calculation $a(0) = 0, a(1) = 1, a(2) = 3, a(3) = 6, a(4) = 10$. Guess a quadratic $a(n) = \alpha n^2 + \beta n + \gamma$ and get the system of equations

$$\{\gamma = 0, \alpha + \beta + \gamma = 1, 4\alpha + 2\beta + \gamma = 3, 9\alpha + 3\beta + \gamma = 6, 16\alpha + 4\beta + \gamma = 10\} \quad ,$$

in the set of variables $\{\alpha, \beta, \gamma\}$. Solving this set of equations yields $\alpha = 1/2$, $\beta = 1/2$ and $\gamma = 0$, that leads us to **conjecture** that $a(n) = (1/2)n^2 + (1/2)n$. Let $b(n) := (1/2)n^2 + (1/2)n$. Now $b(0) = 0$ and

$$b(n) - b(n-1) = (1/2)n^2 + (1/2)n - [(1/2)(n-1)^2 + (1/2)(n-1)] = n \quad .$$

Since both $x(n) = a(n)$ and $x(n) = b(n)$ satisfy $x(0) = 0$ and $x(n) - x(n-1) = n$ it follows that $a(n) \equiv b(n)$. $\square$