Experimental Computation and Visual Theorems

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Abstract. Long before current graphic, visualisation and geometric tools were available, John E. Littlewood (1885-1977) wrote in his delightful *Miscellany*[1]:

> A heavy warning used to be given [by lecturers] that pictures are not rigorous; this has never had its bluff called and has permanently frightened its victims into playing for safety. Some pictures, of course, are not rigorous, but I should say most are (and I use them whenever possible myself). [p. 53]

Over the past five years, the role of visual computing in my own research has expanded dramatically. In part this was made possible by the increasing speed and storage capabilities—and the growing ease of programming—of modern multi-core computing environments.

But, at least as much, it has been driven by my group's paying more active attention to the possibilities for graphing, animating or simulating most mathematical research activities.

Keywords: visual theorems, experimental mathematics, randomness, normality of numbers, short walks, planar walks, fractals, protein confirmation.

1 Introduction

I first briefly discuss what is meant both by *visual theorems* and by *experimental computation*. I then turn to *dynamic geometry* (iterative reflection methods [1]) and *matrix completion problems*[2] (applied to protein confirmation [3]). (See Case studies I and II.) I end with description of recent work from my group in *probability* (behaviour of short random walks [6,8]) and *transcendental number theory* (normality of real numbers [2]). (See Case studies III.)

[1] J.E. Littlewood, *A mathematician's miscellany*, London: Methuen (1953); J. E. Littlewood and Béla Bollobás, ed., *Littlewood's miscellany*, Cambridge University Press, 1986.

[2] See http://www.carma.newcastle.edu.au/jon/Completion.pdf and http://www.carma.newcastle.edu.au/jon/dr-fields11.pptx.

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1.1 Some Early Conclusions: So I Am Sure They Get Made

1. Maths can be done *experimentally*[3] (it is fun) using computer algebra, numerical computation and graphics: SNaG Computations, tables and pictures are experimental data but you can not stop thinking.
2. Making mistakes is fine as long as you learn from them, and keep your eyes open (conquer fear).
3. You can not use what you do not know and what you know you can usually use. Indeed, you do not need to know much before you start research (as we shall see).

2 Visual Theorems and Experimental Mathematics

In a 2012 study *On Proof and Proving* [10] the International Council on Mathematical Instruction wrote:

> The latest developments in computer and video technology have provided a multiplicity of computational and symbolic tools that have rejuvenated mathematics and mathematics education. Two important examples of this revitalization are experimental mathematics and visual theorems.

By a *visual theorem*[4] I mean a picture or animation which gives one confidence that a desired result is true in Gianqunto's sense that it represents "coming to believe it in an independent, reliable, and rational way" (either as discovery or validation) as described in [4]. While we have famous pictorial examples purporting to show all triangle are equilateral, there are equally many or more bogus symbolic proofs that $1 + 1 = 1$. In all cases 'caveat emptor'.

Modern technology properly mastered allows for a much richer set of tools for discovery, validation, and even rigorous proof than our precursors could have ever imagined would come to pass—and it is early days. The same ICMI study [10], quoting [5, p. 1], says enough about the meaning of *experimental mathematics* for our curernet purposes:

> Experimental mathematics is the use of a computer to run computations—sometimes no more than trial-and- error tests—to look for patterns, to identify particular numbers and sequences, to gather evidence in support of specific mathematical assertions that may themselves arise by computational means, including search.
> Like contemporary chemists — and before them the alchemists of old—who mix various substances together in a crucible and heat them to a high temperature to see what happens, today's experimental mathematicians put a hopefully potent mix of numbers, formulas, and algorithms into a computer in the hope that something of interest emerges.

[3] DHB and JMB, "Exploratory Experimentation in Mathematics" (2011), `www.ams.org/notices/201110/rtx111001410p.pdf`

[4] See `http://vis.carma.newcastle.edu.au/`.

3 Case Studies

We turn to three sets of examples:

3.1 Case Study Ia: Iterative Reflections

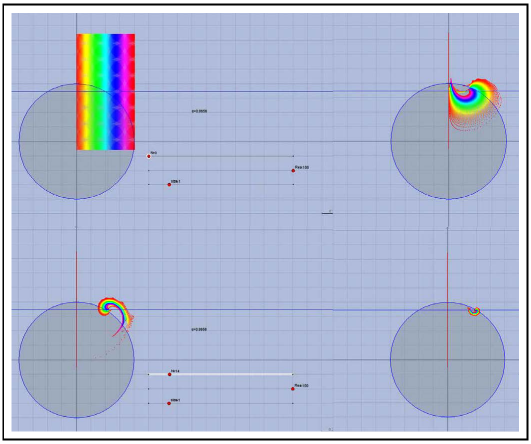
Let $S \subset R^m$. The (nearest point or metric) *projection* onto S is the (set-valued) mapping, $P_S x := \text{argmin}_{s \in S} \|s - x\|$. The *reflection* with respect to S is then the (set-valued) mapping, $R_S := 2P_S - I$. Iterative projection methods have a long and successful history. The basic model [1,3] finds a point in $A \cap B$ assuming information about the projections on A and B is accessible. The corresponding reflection methods are more recent and appear more potent.

Theorem 1 (Douglas–Rachford (1956–1979)). *Suppose $A, B \subset R^m$ are closed and convex. For any $x_0 \in R^m$ define*

$$x_{n+1} := T_{A,B} x_n \text{ where } T_{A,B} := \frac{I + R_B R_A}{2}.$$

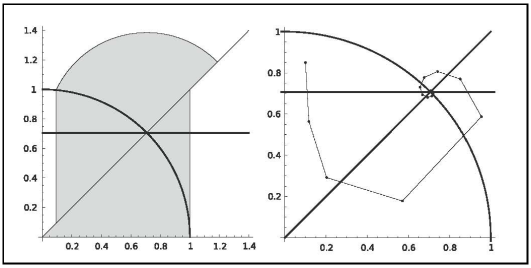
If $A \cap B \neq \emptyset$, then $x_n \to x$ such that $P_A x \in A \cap B$. Else $\|x_n\| \to +\infty$.

The method also applies to a good model for *phase reconstruction*, namely for B affine and A a boundary ‘sphere’. In this case we have some local and many fewer global convergence results; but much empirical evidence— both numeric and geometric (using *Cinderella, Maple* and SAGE).



Cinderella applet[5] showing 20000 starting points coloured by distance from y-axis after $0, 7, 14, 21$ steps. Is this a “*generic* visual theorem” showing global convergence off the (chaotic) y-axis? Note the *error*—scattered red points—from using ‘only’ 14 digit computation.

[5] See `http://carma.newcastle.edu.au/jon/expansion.html`.



Proven region of convergence in grey showing what we can *prove* (L) is less than what we can *see* (R).

3.2 Case Study Ib: Protein Confirmation

Proteins are large biomolecules comprising multiple amino acid chains.[6] Proteins participate in virtually every cellular process and Protein structure → predicts how functions are performed. NMR spectroscopy (Nuclear Overhauser effect[7]) can determine a subset of interatomic distances without damage (under 6Å). This can profitably be viewed as a non-convex *low-rank Euclidean distance matrix completion* problem. We use only interatomic distances below 6Å typically constituting less than 8% of the total nonzero entries of the distance matrix and use our reflection method to extrapolate the rest.

Six Proteins: average (maximum) errors from five replications.

Protein	# Atoms	Rel. Error (dB)	RMSE	Max Error
1PTQ	40	-83.6 (-83.7)	0.0200 (0.0219)	0.0802 (0.0923)
1HOE	581	-72.7 (-69.3)	0.191 (0.257)	2.88 (5.49)
1LFB	641	-47.6 (-45.3)	3.24 (3.53)	21.7 (24.0)
1PHT	988	-60.5 (-58.1)	1.03 (1.18)	12.7 (13.8)
1POA	1067	-49.3 (-48.1)	34.1 (34.3)	81.9 (87.6)
1AX8	1074	-46.7 (-43.5)	9.69 (10.36)	58.6 (62.6)

Here

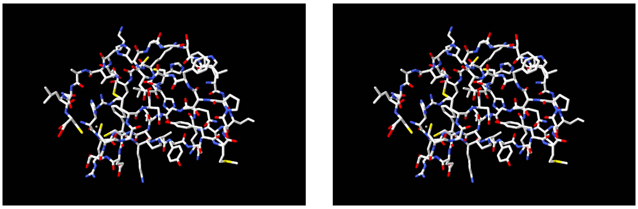
$$\mathrm{Rel.error(dB)} := 10\log_{10}\left(\frac{\|P_{C_2}P_{C_1}X_N - P_{C_1}X_N\|^2}{\|P_{C_1}X_N\|^2}\right),$$

$$\mathrm{RMSE} := \sqrt{\frac{\sum_{i=1}^m \|\hat{p}_i - p_i^{\mathrm{true}}\|_2^2}{\#\mathrm{ofatoms}}}, \qquad \mathrm{Max} := \max_{1\le i\le m} \|\hat{p}_i - p_i^{\mathrm{true}}\|_2.$$

The points $\hat{p}_1, \hat{p}_2, \ldots, \hat{p}_n$ denote the best fitting of $p_1, p_2, \ldots, p_n$ when rotation, translation and reflection is allowed.

The numeric estimates do not well segregate good and poor reconstructions so we ask what the reconstructions *look* like?

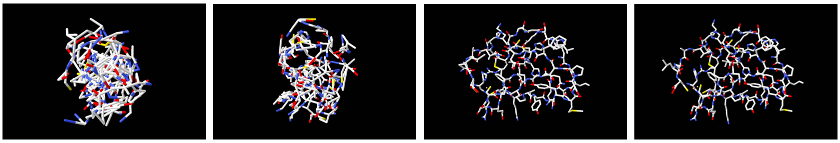
[6] RuBisCO (responsible for photosynthesis) has 550 amino acids (smallish).
[7] A coupling which occurs through space, rather than chemical bonds.



1PTQ (actual) 5,000 steps, -83.6dB (perfect)

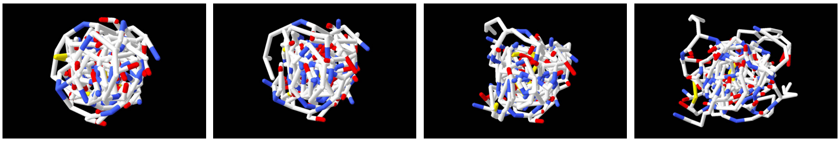
1POA (actual) 5,000 steps, -49.3dB (mainly good!)

The picture of 'failure' suggests many strategies for success. What do reconstructions *look* like?[8] There are many projection methods, so it is fair to ask why we use Douglas-Rachford? The two sets of images below show the striking difference in the two methods.



500 steps, -25 dB. 1,000 steps, -30 dB. 2,000 steps, -51 dB. 5,000 steps, -84 dB.

Douglas–Rachford reflection method reconstruction



500 steps, -22 dB. 1,000 steps, -24 dB. 2,000 steps, -25 dB. 5,000 steps, -28 dB.

Alternating projection method reconstruction

Yet the method of alternating projections works very well for optical abberation correction (originally on the Hubble telescope and now on amateur telescopes attached to latops). And we still struggle to understand why and when these methods work on different convex problems?

3.3 Case Study II: Trefethen's 100 Digit Challenge

In the January 2002 issue of *SIAM News*, Nick Trefethen presented ten diverse problems used in teaching *modern* graduate numerical analysis students at Oxford University, the answer to each being a certain real number. Readers were

[8] Video of the first 3,000 steps of the 1PTQ reconstruction is at `http://carma.newcastle.edu.au/DRmethods/1PTQ.html`.

challenged to compute ten digits of each answer, with a $100 prize to the best entrant. Trefethen wrote, "If anyone gets 50 digits in total, I will be impressed." To his surprise, a total of 94 teams, representing 25 different nations, submitted results. Twenty received a full 100 points (10 correct digits for each problem). Bailey, Fee and I quit at 85 digits! The problems and solutions are dissected most entertainingly in [9]. We shall examine the two final problems.

> **Problem #9**. The integral $I(a) = \int_0^2 [2+\sin(10\alpha)]x^\alpha \sin\left(\frac{\alpha}{2-x}\right)\,\mathrm{d}x$ depends on the parameter α. What is the value $\alpha \in [0,5]$ at which $I(\alpha)$ achieves its maximum?

The maximum α is expressible in terms of a *Meijer-G function*—a special function with a solid history that we use below. While knowledge of this function was not common among contestants, *Mathematica* and *Maple* both will figure this out; help files or a web search then quickly inform the scientist. This is another measure of the changing environment. It is usually a good idea—and not at all immoral—to *data-mine.*

> **Problem #10**. A particle at the center of a 10×1 rectangle undergoes Brownian motion (i.e., 2-D random walk with infinitesimal step lengths) till it hits the boundary. What is the probability that it hits at one of the ends rather than at one of the sides?

Bornemann starts his remarkable solution by exploring *Monte-Carlo methods*, which are shown to be impracticable. A tour through many areas of pure and applied mathematics leads to *elliptic integrals* and *modular functions* which *proves* that the answer is $p = \frac{2}{\pi}\arcsin(k_{100})$ where

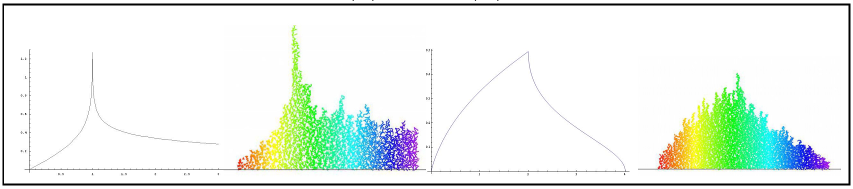
$$k_{100} := \left(\left(3-2\sqrt{2}\right)\left(2+\sqrt{5}\right)\left(-3+\sqrt{10}\right)\left(-\sqrt{2}+\sqrt[4]{5}\right)^2\right)^2,$$

is a *singular value.* [In general $p(a,b) = \frac{2}{\pi}\arcsin\left(k_{(a/b)^2}\right)$.] No one (except harmonic analysts perhaps) anticipated a closed form—let alone one like this. This analysis can be extended to some other shapes, and the computation has been performed by Nathan Cilsby for self-avoiding walks.

3.4 Case Study IIIa: Short Walks

The final set of studies expressedly involve random walks. Our group, motivate initially by multi-dimensional quadrature techniques for higher precision than Monte Carlo can provide looked at the moments and densities of n-step walks of unit size with uniform random angles [6,8]. Intensive numeric-symbolic and graphic computing lead to some striking new results for a century old problem. Here we mention only two. Here p_n is the radial density of the n-step walk ($p_n(x) \sim \frac{2x}{n}e^{-x^2/n}$).

The densities p_3 (L) and p_4 (R) and simulations.



We first discovered $\sigma(x) := \frac{3-x}{1+x}$ is an *involution* on $[0,3]$ ($[0,1] \mapsto [1,3]$):

$$p_3(x) = \frac{4x}{(3-x)(x+1)}\, p_3(\sigma(x)). \tag{1}$$

So $\frac{3}{4}p_3'(0) = p_3(3) = \frac{\sqrt{3}}{2\pi},\ p(1) = \infty$. We then found and proved that:

$$p_3(\alpha) = \frac{2\sqrt{3}\alpha}{\pi\,(3+\alpha^2)}\, {}_2F_1\left(\frac{1}{3}, \frac{2}{3}, 1 \middle| \frac{\alpha^2\,(9-\alpha^2)^2}{(3+\alpha^2)^3}\right) = \frac{2\sqrt{3}}{\pi}\, \frac{\alpha}{\mathrm{AG}_3(3+\alpha^2, 3\,(1-\alpha^2)^{2/3})} \tag{2}$$

where AG_3 is the *cubically convergent* mean iteration (1991): $\mathrm{AG}_3(a,b) := \lim_n a_n = \lim_n b_n$ with $a_{n+1} = \frac{a_n+2b_n}{3}$ and $b_{n+1} = \sqrt[3]{b_n \cdot \frac{a_n^2+a_nb_n+b_n^2}{3}}$, starting with $a_0 = a, b_0 = b$. More surprisingly we ultimately get a modular closed form:

$$p_4(\alpha) = \frac{2}{\pi^2}\, \frac{\sqrt{16-\alpha^2}}{\alpha}\, \mathrm{Re}\, {}_3F_2\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{5}{6}, \frac{7}{6} \middle| \frac{(16-\alpha^2)^3}{108\,\alpha^4}\right). \tag{3}$$

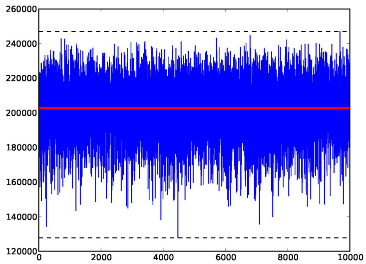
Crucially, for $\mathrm{Re}\, s > -2$ and s not an odd integer the corresponding *moment functions* [6], W_3, W_4 have Meijer-G representations

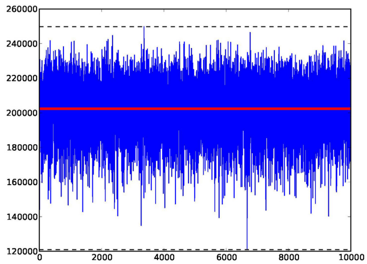
$$W_3(s) = \frac{\Gamma(1+\frac{s}{2})}{\sqrt{\pi}\,\Gamma(-\frac{s}{2})}\, G_{33}^{21}\left(\begin{matrix} 1,1,1 \\ \frac{1}{2}, -\frac{s}{2}, -\frac{s}{2} \end{matrix} \middle| \frac{1}{4}\right),\quad W_4(s) = \frac{2^s}{\pi}\, \frac{\Gamma(1+\frac{s}{2})}{\Gamma(-\frac{s}{2})}\, G_{44}^{22}\left(\begin{matrix} 1, \frac{1-s}{2}, 1, 1 \\ \frac{1}{2} - \frac{s}{2}, -\frac{s}{2}, -\frac{s}{2} \end{matrix} \middle| 1\right).$$

3.5 Case Study IIIb: Number Walks

Our final studies concern representing base-b representations of real numbers as planar walks. For simplicity we consider only binary or hex numbers and use two bits for each direction: 0 = right, 1=up, 2=left, and 3=down [2]. This allows us to compare the statistics of walks on any real number to those for pseudo-random walks[9] of the same length. For now we illustrate only the comparison between the number of points visited by 10,000 million-step pseudo-random walks and for 10 trillion bits of π chopped up into 10,000 walks.

[9] Python uses the *Mersenne Twister* as the core generator. It has a period of $2^{19937} - 1 \approx 10^{6002}$.





Number of points visited by $10,000$ million-step base-4 random walks (L) and π (R)

3.6 Case Study IIIc: Normality of Stoneham Numbers

A real constant α is b-*normal* if, given integer $b \geq 2$, every m-long string of digits appears in the base-b expansion of α with precisely the expected limiting frequency $1/b^m$. Borel showed that almost all irrational real numbers are b-normal in any base but no really explicit numbers (e.g., $e, \pi\sqrt{2}$) have been proven normal. In our final study we shall detail the discovery of the next theorem.

The *Stoneham numbers* are defined by $\alpha_{b,c} = \sum_{n=1}^{\infty} \frac{1}{c^n b^{c^n}}$.

Theorem 2 (Normality of Stoneham constants). *For coprime pairs $b \geq 2, c \geq 2$, the constant $\alpha_{b,c}$ is b-normal, while if $c < b^{c-1}$, $\alpha_{b,c}$ is bc-nonnormal.*

Since $3 < 2^{3-1} = 4, \alpha_{2,3}$ is 2-normal but 6-nonnormal ! This yields the first concrete transcendental to be shown normal in one base yet abnormal in another.

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