Jonathan Borwein: Experimental Mathematician

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Jonathan M. Borwein unexpectedly died on 2 August 2016, in London, Ontario, Canada, where he had been visiting on leave from home institution, the University of Newcastle, Australia.

Since his death, the present author and Nelson H. F. Beebe of the University of Utah have been collecting Borwein's many published papers, books, reports and talks, as well as a number of articles written by others (such as book reviews) about Jon and his work. Our current catalog (available at `http://www.jonborwein.org/jmbpapers/`) lists 1745 items, and the list is certain to grow further. This includes over 500 published books, journal articles and refereed conference papers, a prodigious output for any scholar and especially for a research mathematician. And in an era when many mathematicians focus on a single specialty or subspecialty, Borwein did significant research in a wide range of fields, ranging from analytic number theory and optimization to biomedical imaging, mathematical finance and, especially, experimental mathematics, where he was arguably the world's leader.

1 Pi: A personal remembrance

I confess that I personally became involved in experimental mathematics as a direct result of working with Jonathan Borwein. This stems back to 1984, when I happened to read an article by Jonathan and his brother Peter on how the arithmetic-geometric mean could be utilized to rapidly compute π and the elementary functions [10]. Intrigued by these formulas, I contacted Jonathan and Peter, who sent me some additional formulas for π [12, 13], which I then implemented as part of a test suite for a Cray-2 supercomputer that NASA had just acquired.

One of their formulas is the following: Set $a_0 = 6 - 4\sqrt{2}$, $y_0 = \sqrt{2} - 1$, and

$$\begin{aligned} y_{k+1} &= \frac{1 - (1 - y_k^4)^{1/4}}{1 + (1 - y_k^4)^{1/4}} \\ a_{k+1} &= a_k(1 + y_{k+1})^4 - 2^{2k+3} y_{k+1}(1 + y_{k+1} + y_{k+1}^2). \end{aligned} \tag{1}$$

for $k \geq 0$. Then a_k converge *quartically* to $1/\pi$: each iteration approximately *quadruples* the number of correct digits, provided all iterations are performed to at least the precision required for the result.

In the end, Jonathan, Peter and I co-authored a paper presenting several of these formulas in the historical context of Ramanujan's writings, together with details on how they could be implemented on a computer and what insight one could derive from the results [13]. As a result of this collaboration, I was hooked on experimental mathematics, and have worked in this area, mostly with Jon, ever since. I have since learned that numerous other mathematicians similarly became hooked on experimental mathematics after being introduced to the subject by Jon. He was a masterful salesman for the field.

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Figure 1: Credit: Australian Academy of Science

2 Ramanujan continued fractions

One good example that is illustrative of the experimental methodology that Jon was so fond of can be seen in a pair of papers he wrote with Richard Crandall (who died in December 2012) and Greg Fee on "Ramanujan continued fractions." Given $a, b, \eta > 0$, define

$$R_\eta(a,b) = \cfrac{a}{\eta + \cfrac{b^2}{\eta + \cfrac{4a^2}{\eta + \cfrac{9b^2}{\eta + \ddots}}}}.$$

This continued fraction arises in Ramanujan's *Notebooks*. Ramanujan discovered the beautiful fact that

$$\frac{R_\eta(a,b) + R_\eta(b,a)}{2} = R_\eta\left(\frac{a+b}{2}, \sqrt{ab}\right).$$

Jon had originally wished to record this particular formula in our book *Mathematics by Experiment* [8], but he first wished to computationally check it for validity. An initial attempt to numerically compute $R_1(1,1)$ failed miserably, but with some effort three reliable digits were obtained: $0.693\cdots$, suggesting that this might be $\log 2$. In hindsight, these computations were hindered by the fact that convergence of the fraction is slowest in the simplest case, namely when $a = b$, as in this example.

Nonetheless, it did turn out to be true that $R_1(1,1) = \log 2$, as a special case of the following line of reasoning. From formula (1.11.70) of [9], one can show that for $0 < b < a$,

$$\mathcal{R}_1(a,b) = \frac{\pi}{2}\sum_{n\in \mathrm{Z}} \frac{aK(k)}{K^2(k) + a^2n^2\pi^2}\operatorname{sech}\left(n\pi\frac{K(k')}{K(k)}\right),$$

where $k = b/a = \theta_2^2/\theta_3^2$, $k' = \sqrt{1-k^2}$, K is a complete elliptic integral of the first kind, and θ_2, θ_3 are Jacobian theta functions.

Writing the previous equation as a Riemann sum, one finds that

$$\mathcal{R}(a) = \mathcal{R}_1(a,a) = \int_0^\infty \frac{\operatorname{sech}(\pi x/(2a))}{1+x^2}\,\mathrm{d}x = 2a\sum_{k=1}^\infty \frac{(-1)^{k+1}}{1+(2k-1)a},$$

where the final equality follows from the Cauchy-Lindelof Theorem. This sum may also be written as $\mathcal{R}(a) = \frac{2a}{1+a}F\left(\frac{1}{2a}+\frac{1}{2}, 1; \frac{1}{2a}+\frac{3}{2}; -1\right)$, from which *Maple* or *Mathematica* can be used to compute

$$\mathcal{R}(2) = 0.97499098879872209671990033452 9\ldots.$$

This constant, as written, is difficult to recognize, but if one first divides by $\sqrt{2}$, one can discover, using the *Inverse Symbolic Calculator-2* (`https://isc.carma.newcastle.edu.au`, an online tool that Jon was instrumental in producing and deploying), that the quotient is $\pi/2 - \log(1+\sqrt{2})$. In other words,

$$\mathcal{R}(2) = \sqrt{2}\left[\pi/2 - \log(1+\sqrt{2})\right].$$

From this specific experimental evaluation, Borwein, Crandall and Fee were led to conjecture and then prove the general formula

$$\mathcal{R}(a) = 2\int_0^1 \frac{t^{1/a}}{1+t^2}\,\mathrm{d}t,$$

from which it trivially follows that $\mathcal{R}(1) = \log 2$. See [14, 15, 9] for additional details.

3 Ising integrals

Another good illustration of Jon's experimental methodology in action was his analysis (in conjunction with Richard Crandall and myself) [2] of the following three classes of integrals that arise in mathematical physics: C_n are connected to quantum field theory, D_n arise in Ising theory, while the E_n integrands are derived from D_n:

$$C_n := \frac{4}{n!}\int_0^\infty \cdots \int_0^\infty \frac{1}{\left(\sum_{j=1}^n (u_j + 1/u_j)\right)^2} \frac{\mathrm{d}u_1}{u_1} \cdots \frac{\mathrm{d}u_n}{u_n}$$

$$D_n := \frac{4}{n!}\int_0^\infty \cdots \int_0^\infty \frac{\prod_{i<j}\left(\frac{u_i-u_j}{u_i+u_j}\right)^2}{\left(\sum_{j=1}^n (u_j + 1/u_j)\right)^2} \frac{\mathrm{d}u_1}{u_1} \cdots \frac{\mathrm{d}u_n}{u_n}$$

$$E_n = 2\int_0^1 \cdots \int_0^1 \left(\prod_{1\le j<k\le n} \frac{u_k - u_j}{u_k + u_j}\right)^2 \mathrm{d}t_2\, dt_3 \cdots \mathrm{d}t_n,$$

where in the last line $u_k = t_1 t_2 \cdots t_k$.

One early observation was that the C_n integrals can be converted to one-dimensional integrals involving the modified Bessel function $K_0(t)$:

$$C_n = \frac{2^n}{n!}\int_0^\infty t K_0^n(t)\ \mathrm{d}t.$$

Upon computing high-precision numerical values of these integrals, using the tanh-sinh quadrature algorithm [1], it quickly became apparent that these values approach a limit. For example:

$$C_{1024} = 0.6304735033743867961220401927108789043545870787\ldots$$

The online Inverse Symbolic Calculator-2, mentioned above, quickly identified this value as

$$\lim_{n\to\infty} C_n = 2e^{-2\gamma},$$

where γ denotes Euler's constant, a result which was then proved.

Subsequently we utilized high-precision computations (which in some cases required a highly parallel supercomputer), in conjunction with Ferguson's PSLQ algorithm [17, 6], to find experimental evaluations of other specific instances of these integrals, including:

$$\begin{aligned}
D_3 &= 8 + 4\pi^2/3 - 27\,\mathrm{L}_{-3}(2)\\
D_4 &= 4\pi^2/9 - 1/6 - 7\zeta(3)/2\\
E_2 &= 6 - 8\log 2\\
E_3 &= 10 - 2\pi^2 - 8\log 2 + 32\log^2 2\\
E_4 &= 22 - 82\zeta(3) - 24\log 2 + 176\log^2 2 - 256(\log^3 2)/3 + 16\pi^2\log 2 - 22\pi^2/3\\
E_5 &= 42 - 1984\,\mathrm{Li}_4(1/2) + 189\pi^4/10 - 74\zeta(3) - 1272\zeta(3)\log 2 + 40\pi^2\log^2 2\\
&\quad - 62\pi^2/3 + 40(\pi^2\log 2)/3 + 88\log^4 2 + 464\log^2 2 - 40\log 2,
\end{aligned}$$

where $\mathrm{L}_{-3}(2)$ is a Dirichlet L-function constant, $\zeta(x)$ is the Riemann zeta function and $\mathrm{Li}_n(x)$ is the polylogarithm function. The formula for E_5, which was initially found by Borwein (and which he was quite proud of), remained a numerically discovered but open conjecture for several years, but was finally proven in 2014 by Erik Panzer [18]. Resolution of the general case is still open.

4 Algebraic numbers in Poisson potential functions

One final example that we will mention here arose when Richard Crandall, who was studying lattice sums associated with the Poisson equation, in connection with a technique to sharpen photographic images, brought to Jon's attention the sums

$$\phi_n(r_1, \ldots, r_n) = \frac{1}{\pi^2} \sum_{m_1, \ldots, m_n \text{ odd}} \frac{e^{i\pi(m_1 r_1 + \cdots + m_n r_n)}}{m_1^2 + \cdots + m_n^2}.$$

After extensive analysis and numerical experimentation [3, 4, 5], Jon and Richard, later including myself and Jon Zucker, discovered the intriguing fact that when x and y are rational,

$$\phi_2(x, y) = \frac{1}{\pi} \log A,$$

where A is an *algebraic number* that depends on the particular values of x and y.

A key breakthrough here, due to Jon, was to observe that the $\phi_2(x, y)$ function could be numerically computed much more rapidly as follows [3]:

$$\phi_2(x, y) = \frac{1}{2\pi} \log \left| \frac{\theta_2(z, q)\theta_4(z, q)}{\theta_1(z, q)\theta_3(z, q)} \right|,$$

where $q = e^{-\pi}$ and $z = \frac{\pi}{2}(y + ix)$. The four theta functions in turn can be computed as [11, p. 52]:

$$\begin{aligned}
\theta_1(z, q) &= 2 \sum_{k=1}^{\infty} (-1)^{k-1} q^{(2k-1)^2/4} \sin((2k-1)z), \\
\theta_2(z, q) &= 2 \sum_{k=1}^{\infty} q^{(2k-1)^2/4} \cos((2k-1)z), \\
\theta_3(z, q) &= 1 + 2 \sum_{k=1}^{\infty} q^{k^2} \cos(2kz), \\
\theta_4(z, q) &= 1 + 2 \sum_{k=1}^{\infty} (-1)^k q^{k^2} \cos(2kz).
\end{aligned}$$

In our experiments using these formulas, we computed $\alpha = A^8 = \exp(8\pi\phi_2(x, y))$ for various specific rationals x and y. Then we generated the vector $(1, \alpha, \alpha^2, \cdots, \alpha^d)$ as input to a program implementing the three-level multipair PSLQ program [17, 6]. When successful, the program returned the vector of integer coefficients $(a_0, a_1, a_2, \cdots, a_d)$ of a polynomial satisfied by α as output. With some experimentation on the degree d, and after symbolic verification using *Mathematica*, we were able to ensure that the resulting polynomial is in fact the minimal polynomial satisfied by α. Table 1 shows some examples of these computational results [3].

After these results were first obtained, Jason Kimberley, a graduate student at the University of Newcastle, Australia, observed that the degree $m(s)$ of the minimal polynomial associated with the case $x = y = 1/s$ appears to be given by the following formula. Set $m(2) = 1/2$. Otherwise for primes p congruent to 1 modulo 4, set $m(p) = (p-1)^2/4$, and for primes p congruent to 3 modulo 4, set $m(p) = (p^2-1)/4$. Then for any other positive integer s whose prime factorization is $s = p_1^{e_1} p_2^{e_2} \cdots p_r^{e_r}$,

$$m(s) = 4^{r-1} \prod_{i=1}^{r} p_i^{2(e_i-1)} m(p_i). \qquad (2)$$

s	Minimal polynomial corresponding to $x = y = 1/s$:
5	$1 + 52\alpha - 26\alpha^2 - 12\alpha^3 + \alpha^4$
6	$1 - 28\alpha + 6\alpha^2 - 28\alpha^3 + \alpha^4$
7	$-1 - 196\alpha + 1302\alpha^2 - 14756\alpha^3 + 15673\alpha^4 + 42168\alpha^5 - 111916\alpha^6 + 82264\alpha^7$ $-35231\alpha^8 + 19852\alpha^9 - 2954\alpha^{10} - 308\alpha^{11} + 7\alpha^{12}$
8	$1 - 88\alpha + 92\alpha^2 - 872\alpha^3 + 1990\alpha^4 - 872\alpha^5 + 92\alpha^6 - 88\alpha^7 + \alpha^8$
9	$-1 - 534\alpha + 10923\alpha^2 - 342864\alpha^3 + 2304684\alpha^4 - 7820712\alpha^5 + 13729068\alpha^6$ $-22321584\alpha^7 + 39775986\alpha^8 - 44431044\alpha^9 + 19899882\alpha^{10} + 3546576\alpha^{11}$ $-8458020\alpha^{12} + 4009176\alpha^{13} - 273348\alpha^{14} + 121392\alpha^{15}$ $-11385\alpha^{16} - 342\alpha^{17} + 3\alpha^{18}$
10	$1 - 216\alpha + 860\alpha^2 - 744\alpha^3 + 454\alpha^4 - 744\alpha^5 + 860\alpha^6 - 216\alpha^7 + \alpha^8$

Table 1: Sample of polynomials produced in earlier study [3].

This sequence now appears as `http://oeis.org/A218147` in the *Online Encyclopedia of Integer Sequences*. Does Kimberley's formula hold for any or all higher s?

We then explored these polynomials using significantly more powerful computational tools, including a new, more advanced high-precision computation package, a new three-level multipair PSLQ program, and an implementation on a parallel computer system [5]. With this improved capability (more than 150 times faster than before), we confirmed that Kimberley's formula holds for all integers s up to 52, except for a handful that were too expensive to test, and also for $s = 60$ and $s = 64$. These computations were very challenging, requiring up to 64,000-digit precision, producing polynomials with degrees up to 512 and integer coefficients up to 10^{229}.

By examining the computed results, and, quite literally, doing Google searches on some of the resulting polynomial coefficients, we found connections to a sequence of polynomials defined in a 2010 paper by Savin and Quarfoot [19]. These investigations subsequently led to a proof, by Watson Ladd of the University of California, Berkeley, of Kimberley's formula and also the fact that when s is even, the corresponding polynomial is palindromic [5].

Needless to say, Jon was very pleased with this most satisfying conclusion to a problem that initially appeared to be intractable. Sadly, he died before the paper documenting these results appeared in *Experimental Mathematics* [5].

5 Conclusion

Jonathan Borwein's leadership and prodigious output in experimental mathematics (and also in optimization) is a singular contribution to modern mathematics. Among other things, his devoted service as an editor for *Experimental Mathematics* will be sorely missed.

But beyond his technical accomplishments, he was a master of mathematical communication, mathematical education, and in promoting science, mathematics and computing to the general public. To this end, Jon wrote and lectured tirelessly. By one reckoning he presented an average of one lecture per week for decades, and wrote over 100 articles targeted to the general public. His death is a loss to all those who treasure modern mathematics, science and clear thinking.

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