New computations of Poisson polynomials: An application of very high-precision floating-point arithmetic

> David H. Bailey http://www.davidhbailey.com Lawrence Berkeley National Lab (retired)

> > July 3, 2023

Polynomials arising from the Poisson potential function

The Poisson potential function appears in numerous applied math contexts, ranging from mathematical physics to sharpening iPhone images. A simple 2-D instance is:

$$\phi_2(x,y) = rac{1}{\pi^2} \sum_{m,n ext{ odd}} rac{\cos(m\pi x)\cos(n\pi y)}{m^2 + n^2}$$

A 2013 study numerically discovered and then proved the intriguing fact that when x and y are rational, then $\phi_2(x, y)$ satisfies

$$\phi_2(x,y) = rac{1}{\pi} \log eta(x,y)$$

where $\beta(x, y)$ is algebraic, i.e., the root of an integer polynomial of some degree m.

By computing high-precision numerical values of $\phi_2(x, y)$ for various specific rational x and y, and applying variants of the PSLQ program, we were able to produce the explicit minimal polynomials for α in several simple specific cases.

D. H. Bailey, J. M. Borwein, R. E. Crandall and J. Zucker, "Lattice sums arising from the Poisson equation," *Journal of Physics A: Mathematical and Theoretical*, vol. 46 (2013), 115201.

Key breakthrough: Borwein's fast algorithm to compute $\phi_2(x, y)$

The original formula for $\phi_2(x, y)$ converges much too slowly for numerical evaluation. But this formula, found by Jonathan Borwein (deceased 2016), is remarkably efficient:

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

where $q = e^{-\pi}$ and $z = \frac{\pi}{2}(y + ix)$. Note that these series converge very rapidly:

$$egin{aligned} & heta_1(z,q)=2\sum_{k=1}^\infty(-1)^{k-1}q^{(2k-1)^2/4}\sin((2k-1)z),\ & heta_2(z,q)=2\sum_{k=1}^\infty q^{(2k-1)^2/4}\cos((2k-1)z),\ & heta_3(z,q)=1+2\sum_{k=1}^\infty q^{k^2}\cos(2kz),\ & heta_4(z,q)=1+2\sum_{k=1}^\infty(-1)^kq^{k^2}\cos(2kz). \end{aligned}$$

The PSLQ integer relation algorithm

Let $X = (x_k)$ be an (m + 1)-long real or complex vector. An integer relation algorithm finds a nontrivial integer vector $A = (a_k)$ such that

 $a_0x_0+a_1x_1+\cdots+a_mx_m = 0.$

- The PSLQ algorithm and the multipair PSLQ algorithm are commonly used for integer relation detection. Variants of the LLL algorithm can also be used.
- ▶ Integer relation detection requires very high precision floating-point arithmetic: at least $(m + 1) \cdot \max_k \log_{10} |a_k|$ digits (typically hundreds or thousands of digits), both in the input data and the algorithm, or else the true relation will be lost in a sea of numerical artifacts.
- Fast variations of PSLQ and multipair PSLQ utilize two, three or even four levels of precision, doing as much computation as possible with only double precision, and switching to higher levels only when needed.

D. H. Bailey and D. J. Broadhurst, "Parallel integer relation detection: Techniques and applications," *Mathematics of Computation*, vol. 70, no. 236 (Oct 2000), 1719–1736.

Numerically finding minimal polynomials using PSLQ

Integer relation algorithms can be used to recognize a computed numerical value as the root of an integer polynomial of degree m.

Example: α is suspected to be an algebraic number of degree 8 or less:

 $\alpha = 2.1195912698291751313298483349346871106280\ldots$

What is its minimal polynomial?

Method: Compute the vector $(1, \alpha, \alpha^2, \dots, \alpha^8)$, then apply a variant of the PSLQ algorithm. This produces the integer vector (1, -216, 860, -744, 454, -744, 860, -216, 1), so that α appears to satisfy the polynomial:

$$0 = 1 - 216\alpha + 860\alpha^2 - 744\alpha^3 + 454\alpha^4 - 744\alpha^5 + 860\alpha^6 - 216\alpha^7 + \alpha^8$$

High-level computational algorithm

- 1. Given rationals x = p/s and y = q/s, select a conjectured minimal polynomial degree *m*, precision levels P_1 and P_2 and other parameters for the run.
- Calculate φ₂(x, y) to P₂-digit precision using Borwein's fast algorithm. When done, calculate α = exp(8πφ₂(x, y)) and generate the (m + 1)-long vector x = (1, α, α², ···, α^m), to P₂-digit precision. Note: the polynomials are simpler in terms of α = (β(x, y))⁸ = exp(8πφ₂(x, y)).
- 3. Apply a variant of the PSLQ algorithm to find an integer relation for x.
- 4. If no numerically significant relation is found, try again with a larger degree *m* or higher precision. If a relation is found, employ *Mathematica* or *Maple* to ensure that the polynomial is irreducible. Alternatively, rerun the problem with the degree *m* reduced by one, to ensure that no numerically significant relation is found with this smaller degree.

2013: Some initial Poisson polynomial computations

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

Questions:

- Given *s*, what is the degree of the corresponding minimal polynomial?
- Note that when s is even, the polynomial is palindromic, i.e., coefficients $a_k = a_{m-k}$. Does this pattern hold for all even s?

These computations were very expensive and required very high precision. Help! More powerful computational tools are required.

Kimberley's formula for the degree of the polynomial

Based on these preliminary results, Jason Kimberley of 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 rule:

Set m(2) = 1/2. Otherwise for primes p congruent to 1 mod 4, set $m(p) = int^2(p/2)$, where int denotes greatest integer, and for primes p congruent to 3 mod 4, set m(p) = int(p/2)(int(p/2) + 1). Then for any other positive integer s whose prime factorization is $s = p_1^{e_1} p_2^{e_2} \cdots p_r^{e_r}$,

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

Questions:

- Does Kimberley's formula hold for larger s?
- Does the palindromic property hold for larger even s?

2016: Improvements to the Poisson polynomial program

- 1. A new thread-safe arbitrary precision floating-point package.
- 2. Multiprecision software may optionally utilize the MPFR / GMP packages for even faster performance.
- 3. A new 3-level multipair PSLQ program, up to 5X faster:
 - a Double precision (appr. 15 digit accuracy).
 - b Medium multiprecision: varies from 100 digits to 1200 digits on Poisson problems.
 - c Full multiprecision: varies from 2,500 digits to 50,000 digits on Poisson problems.
- 4. Faster hardware: an 8-core MacPro system with Intel processor.

D. H. Bailey, J. M. Borwein, J. Kimberley and W. Ladd, "Computer discovery and analysis of large Poisson polynomials," *Experimental Mathematics*, 27 Aug 2016, vol. 26, 349-363, https://www.davidhbailey.com/dhbpapers/poisson-res.pdf.

Degree-100 minimal polynomial found for the case x = y = 1/25

- 283348778825 o* - 56060293400080 A* -562W11150130800 // -1906195067754657491760 a¹¹ - 256411500002006643010482000 0 - 256411580098396643830482000 α⁻¹ + 1386200356872030954311366400 α⁻³ +1346700356872030464211266403 0* +0088870483476589306411065750 0* 73358806455331763836484382500 -7135990545511176393649618250003 a** - 38212880291083155937295195441746800 m² 74032065945345967753102951351295900 or + 3685570175103433750838888367333133608 cc - 20955 791751024 737508 3939835 7021130508 a - 175855808985 77538033683566583501380300 a² — 17580580809577528033993599683501290200 α
> 74852710235773360685353353982788556000 α +594175511524312220492120757310324404000 Δ** -12004812017258602359378600176026068058456 Δ** +29340961737653182271816694472006500014100 a²¹ + 394 388553221080980775811796973709891661972 cc - 105077311003132210808007798117908787878989100097213 95560391964393397280402140487430432508004900 or - 202305336551868593336977017479411555696276960 cr - 5250613909211822290611229001896018960180091290304 cc — 454264602288840080028112470380711412629425500 is ± 333.89561099972574095810639259223345183420000 is - 451584154001204338877039495371276398657115 + 2655821534372089246354523887715099696938068 - 4 - 127 2765 122 400 104850 541 9427 4127 224067 210 + 524 2055 20985 1537 7367 40795654621 634056 2900 \alpha - 3264527861365792560817221584358055000 + 47236099216856361844453309451178900 co -178858482702935977506858126791577500 a -15898883.0972285544578912251280 +1778153714893883182147476433 c -134561774900933536521588000 c - 3011302/31114411241540400 a 122000003990534 - 110611006665 +13995250.0*

+6700 0 **

Palindromic polynomials

From our results, in the case x = 1/s, y = 1/s where s is even, the resulting polynomial is always palindromic $(a_k = a_{m-k})$. For instance, when s = 16, $p_{16}(\alpha) = 1 - 1376\alpha^{1} - 12560\alpha^{2} - 3550496\alpha^{3} + 81241720\alpha^{4} - 169589984\alpha^{5}$ $+ 1334964944 \alpha^{6} - 24307725984 \alpha^{7} + 238934926108 \alpha^{8} - 1043027124704 \alpha^{9}$ $+2328675366384 \alpha^{10} - 3219896325280 \alpha^{11} + 4238551472456 \alpha^{12}$ $- 10247414430048 \alpha^{13} + 28552105805904 \alpha^{14} - 55832851687968 \alpha^{15}$ $+70020268309062\alpha^{16}$ $- \, 55832851687968 \alpha^{17} + 28552105805904 \alpha^{18} - 10247414430048 \alpha^{19}$ $+4238551472456\alpha^{20} - 3219896325280\alpha^{21} + 2328675366384\alpha^{22}$ $- 1043027124704 \alpha^{23} + 238934926108 \alpha^{24} - 24307725984 \alpha^{25} + 1334964944 \alpha^{26}$ $- 169589984 \alpha^{27} + 81241720 \alpha^{28} - 3550496 \alpha^{29} - 12560 \alpha^{30} - 1376 \alpha^{31} + \alpha^{32}$

Nitya Mani, a student at Stanford University, pointed out that if α is a root of a palindromic polynomial such as this, then $\alpha + 1/\alpha$ is a root of a transformed polynomial of half the degree. This fact has been used to *greatly* accelerate the computation of Poisson polynomials when *s* is an even integer.

2016: A proof of Kimberley formula for the case x = 1/s, y = 1/s

Some observations from the polynomials produced by the program:

- The algebraic number α_s is the *largest* real root of the associated polynomial.
- The polynomial has $\varphi(s)$ real roots, where φ is the Euler totient function.
- Roots are connected to a sequence of polynomials defined in a 2010 paper by Savin and Quarfoot of the University of Utah, which was found by doing an Google search for "387221579866," a coefficient of the polynomial for the case (1/11, 1/11).

These observations ultimately led to a proof, by Watson Ladd of U.C. Berkeley, of Kimberley's formula and also the palindromic property, in the specific case x = y = 1/s.

D. H. Bailey, J. M. Borwein, J. Kimberley and W. Ladd, "Computer discovery and analysis of large Poisson polynomials," *Experimental Mathematics*, 27 Aug 2016, vol. 26, 349–363, https://www.davidhbailey.com/dhbpapers/poisson-res.pdf.

What about the many cases with $x \neq y$?

All of the computations and results mentioned above are for the case x = y = 1/s for some positive integer *s*.

What about rationals x = p/s, y = q/s, with $p \neq q$? Initial results indicated that Kimberley's formula does not hold for these more general rationals.

Is there a generalization of Kimberley's formula that holds in these other cases? Does the palindromic property hold for these other cases?

To address this more general problem requires many times more computation than for the x = y = 1/s cases.

A familiar refrain: Help! More powerful computational tools are required.

2022: New computational tools for Poisson polynomials

- 1. A new high-level multiprecision package, based on integer arithmetic, that is approximately 3X faster than before, nearly as fast as using MPFR / GMP.
- 2. A new 4-level multipair PSLQ program:
 - a Double precision (approx. 15 digit accuracy).
 - b Quad precision (approx. 32 digit accuracy).
 - c Medium multiprecision: varies from 100 digits to 1200 digits on Poisson problems.
 - d Full multiprecision: varies from 2500 digits to 100,000 digits on Poisson problems.
- 3. The code does as much computation as possible in double precision; automatically shifts to higher precision when required (very challenging to reliably program).
- 4. Faster hardware: A 10-core MacStudio, with Apple's low-power M1 Pro processor, thus mercifully helping the author avoid bankruptcy from electric bills.

2023: New computer runs

- ▶ The new software has been used to compute the minimal polynomials for the entire set of cases (p/s, q/s), where $1 \le p \le q < s/2$ and $10 \le s \le 36$, and also for s = 38, 40, 42 and s = 50 (a total of 2206 cases).
- These runs required up to 32,000-digit floating-point arithmetic and thousands of processor-core hours run time.

Results: The following modification of Kimberley's formula appears to hold in all cases $(1 \le p \le q < s/2 \text{ and } gcd(p, q, s) = 1)$:

- 1. For the cases x = y = p/s, Kimberley's formula holds; further, for fixed *s*, all these cases share the same minimal polynomial).
- 2. For the cases x = p/s, y = q/s with s odd, Kimberley's formula holds (except for a few where the correct degree is half Kimberley's rule).
- 3. For the cases x = p/s, y = q/s, with s even and both p and q odd, Kimberley's formula holds (except for a few where the correct degree is half Kimberley's rule).
- 4. For the cases x = p/s, y = q/s, with s even and one of p or q is even, the correct degree is twice Kimberley's formula (except for a few where the correct degree is equal to Kimberley's rule).

Sharing of minimal polynomials

One intriguing finding from the latest computations is that many cases for a given s share the same minimal polynomial, even though the α numerical values are different.

For example, when s = 17, the (x, y) cases (1/17, 1/17), (2/17, 2/17), (3/17, 3/17), (5/17, 5/17), (6/17, 6/17), (7/17, 7/17), (8/17, 8/17) all satisfy the same degree-64 minimal polynomial:

 $+ 1 + 6912\alpha^{1} - 1023008\alpha^{2} + 535196800\alpha^{3} + 7742027760\alpha^{4} - 2451239864832\alpha^{5} + 14026465723552\alpha^{6} - 2494265652888704\alpha^{7} + 1845344552215032\alpha^{8} + 21614293158955264\alpha^{9} - 1840469978381611680\alpha^{10} + 26560170568288794240\alpha^{11} - 219265475764921569840\alpha^{12} + 1143759465759937297408\alpha^{13} - 4563932639248948435424\alpha^{14} + 21048406812137688311168\alpha^{15} - 123756069205191278016740\alpha^{16} + 662708878348907477250816\alpha^{17} - 2671051287612630032421280\alpha^{18} + 7693234584556635821267584\alpha^{19} - 14862548097474240887146768\alpha^{20} + 1198543909280968199200248\alpha^{21} + 44351668349396581870408736\alpha^{22} - 259625664937972467300807296\alpha^{23} + 80318611589967670394823864\alpha^{24} - 1789602095389051533149533952\alpha^{23} + 305552833334008777605289376\alpha^{26} - 4156271487999506323835036544\alpha^{27} + 490396367671959157531751248\alpha^{28} - 6019517253583562192139109888\alpha^{29} + 6780067564346216307831284640\alpha^{30} - 13334548483907481046238812288\alpha^{11} + 1736285748941944863086629318\alpha^{23} - 17358556296005992180018969\alpha^{33} + 11966489230110362129440701856\alpha^{34} - 3898113922387426442055756416\alpha^{35} - 245198393972767054540629348\alpha^{36} + 47344659105587746050587136\alpha^{47} - 38818186944576966609727674704\alpha^{31} + 210149293730991177681793664\alpha^{39} - 83007484081366960661051352\alpha^{40} + 2693667927571630303787494\alpha^{41} - 965965751150818427483040\alpha^{42} + 4631153272057913438161792\alpha^{43} - 221556725767373192657168\alpha^{44} + 815378330335140369288294\alpha^{45} - 2079969173966458311379616\alpha^{46} + 331427117746835861477504\alpha^{47} - 188555288875733014756\alpha^{49} - 221556725767373192657168\alpha^{44} + 815378330335140369288294\alpha^{45} - 2079969173966458311379616\alpha^{46} + 331427117746835861477504\alpha^{47} - 188555288875733014756\alpha^{49} - 2355228650835616208\alpha^{49} + 329260902507960858656\alpha^{50} - 73883647673944491136\alpha^{51} + 76552613117134517712\alpha^{52} - 1424154241008650752\alpha^{53} + 342676113911934816\alpha^{54} - 507040\alpha^{56} - 125943824\alpha^{66} + 62013440\alpha^{61} - 670240\alpha^{52} - 1408\alpha^{64} + 13078450616\alpha^{66} - 154854254425344\alpha^{57} - 3704022772520\alpha^{59} + 404224147840\alpha^{59} - 125943824\alpha^{66} + 6201$

July 2023: New results: The Poisson ψ function

The 2013 study mentioned the closely related function

$$\psi_2(x, y) = rac{1}{\pi^2} \sum_{m, n \text{ even}} rac{\cos(\pi m x) \cos(\pi n y)}{m^2 + n^2}$$

As with $\phi_2(x, y)$, the authors found that when x and y are rational, then $\psi_2(x, y) = 1/\pi \cdot \log(\beta(x, y))$, for algebraic $\beta(x, y)$.

As the present study was being concluded, DHB discovered formulas and computational techniques to find minimal polynomials for $\psi_2(x, y)$. Intriguing initial results have been obtained.

However, the computations and analysis here are significantly more challenging than with $\phi_2(x, y)$, requiring, among other things, much higher precision — up to 100,000-digit or more floating-point arithmetic even for modest-sized *s*.

Details will be provided in a separate report.

Conclusions

- New software has been used to compute the minimal polynomials for α corresponding to φ₂(x, y), for a total of 2206 cases. These runs required up to 32,000-digit floating-point and several CPU-months run time.
- ► A modification of Kimberley's formula appears to hold in all cases, although no proof is known. For a given *s*, many cases share the same minimal polynomial.
- Exploring 3-D Poisson polynomials and polynomials associated with $\psi_2(x, y)$ will require much more computation, with even higher levels of numeric precision (100,000 or more digits).
- ► A familiar refrain: Help! More powerful computational tools are required.

This talk is available at https://www.davidhbailey.com/dhbtalks/dhb-fpt-2023.pdf.

Full results are available at https://www.davidhbailey.com/dhbpapers/poisson-2023.pdf.