Empirically studying half-integral weight modular forms

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This reflects a collaboration with Mehmet Kıral, Li-Mei Lim, and Thomas Hulse. (But all mistakes are probably my own).

I should also thank BU and MIT for providing many, many CPU cycles to this project.

The Selberg Class

Typical L-functions

Half-integral weight modular forms

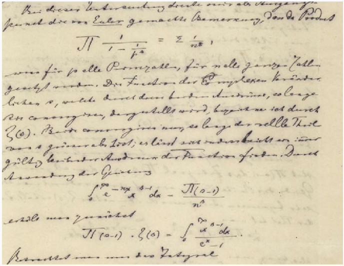
Computational Results and Methodology

Riemann Zeta

The prototypical classical L-function is

$$\zeta(s) = \sum_{n \geq 1} \frac{1}{n^s} = \prod_p \left(1 - \frac{1}{p^s}\right)^{-1},$$

which converges (and is originally defined) for $\operatorname{Re} s > 1$, but which can be meromorphically continued to $\mathbb{C}$.



Riemann's notes introducing $\zeta(s)$ around 1859

The *completed* zeta function

$$\Lambda(s) := \pi^{-\frac{s}{2}} \Gamma\left(\tfrac{s}{2}\right) \zeta(s)$$

satisfies a functional equation

$$\Lambda(s) = \Lambda(1 - s).$$

Riemann introduced $\zeta(s)$ to study questions about the distribution and count of primes. To prove the Prime Number Theorem ($\pi(X) \sim X/\log X$), you consider a Mellin transform

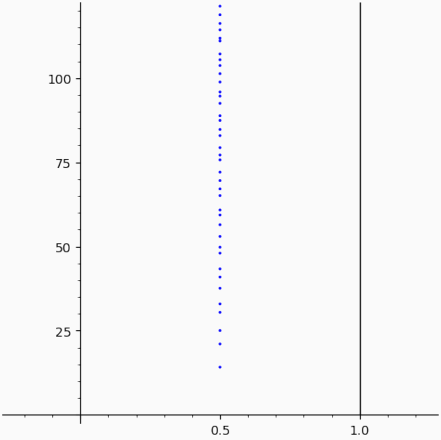
$$\frac{1}{2\pi i}\int_{2-i\infty}^{2+i\infty} \frac{\zeta'(s)}{\zeta(s)}\frac{X^s}{s}\,ds \tag{1}$$

and apply tools and methods from complex analysis.

The connection with primes is apparent from the Euler product

$$\zeta(s) = \prod_p \left(1 - \frac{1}{p^s}\right)^{-1}.$$

Error terms in this proof of the Prime Number Theorem are related to zeros of $\zeta(s)$, as can be seen from (1).



These are the zeros (with $0 < \operatorname{Im} s < 125$) of $\zeta(s)$ in the critical strip. The smallest zero has imaginary part $14.1347\ldots$

The Riemann Hypothesis is that all (nontrivial) zeros of $\zeta(s)$ are on this line.

The Selberg Class of L-functions

More generally, we frequently study the Selberg Class of L-functions. These are Dirichlet series

$$L(s) = \sum_{n \geq 1} \frac{a(n)}{n^s}$$

that satisfy

1. **Analytic Continuation**: $L(s)$ has analytic continuation to $\mathbb{C}$ (with the possible exception of a pole at $s = 1$).
2. **Ramanujan Conjecture**: The coefficients grow slowly, $|a(n)| \ll n^{\epsilon}$ for any $\epsilon > 0$.
3. **Functional Equation**: $L(s)$ can be completed $\Lambda(s) = L(s) Q^s G(s)$ for a (real) number Q and a product of Gamma factors $G(s)$, such that $\Lambda(s) = \epsilon \overline{\Lambda(1 - \overline{s})}$ for some $|\epsilon| = 1$.
4. **Euler Product**: $L(s)$ has an Euler product $L(s) = \prod_p L_p(s)$ for "nice" objects $L_p(s)$.

It turns out that to many objects of arithmetic interest, we can associate an L-function that is (perhaps conjecturally) in the Selberg Class. And all of these L-functions are conjectured to satisfy similar properties to the $\zeta(s)$.

For example, a Generalized Riemann Hypothesis is conjectured for Selberg Class L-functions: all (nontrivial) zeros of $L(s)$ should be on the line $\operatorname{Re} s = \frac{1}{2}$.

Modular L-functions

One source of L-functions are modular forms. A (weight k, holomorphic) modular form is a holomorphic function f on the upper half-plane $\mathcal{H} = \{x + iy : (x, y) \in \mathbb{R}^2, y > 0\}$, which transforms in a prescribed way under the action of a matrix group $\Gamma \subseteq \mathrm{SL}(2, \mathbb{Z})$:

$$f(\gamma z) := f\left(\frac{az+b}{cz+d}\right) = (cz+d)^k f(z), \qquad \gamma = \left(\begin{smallmatrix} a & b \\ c & d \end{smallmatrix}\right) \in \Gamma \subseteq \mathrm{SL}(2, \mathbb{Z}).$$

Further, we require $f(z)$ to be holomorphic on the compactified quotient $\Gamma \backslash \mathcal{H}$, which translates to f having a Fourier expansion

$$f(z) = \sum_{n \geq 0} a(n) e(nz) \qquad e(z) := e^{2\pi i z},$$

(and a few other well-behaved Fourier expansions associated to other cusps of $\Gamma \backslash \mathcal{H}$).

If the Fourier expansions associated to f have zero constant coefficient

$$f(z) = \sum_{n \geq 1} a(n) e(nz),$$

then f is called a holomorphic cuspform. Modular cuspforms of weight k associated to Γ form a vector space, which we denote by $S_k(\Gamma)$.

There is an infinite family of Hecke operators T_p, indexed by primes, that act linearly on $S_k(\Gamma)$. There is a basis of $S_k(\Gamma)$ that consists of cuspforms that are simultaneous eigenforms for all of the Hecke operators. Normalized appropriately, the coefficient $a(p)$ is the eigenvalue of f of the Hecke operator T_p, and the action of the Hecke operators implies that the coefficients are multiplicative.

To each normalized cuspidal modular Hecke eigenform f, we can associate an L-function

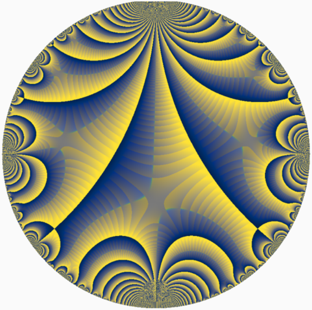
$$L(s, f) = \sum_{n \geq 1} \frac{a(n)}{n^{s + \frac{k-1}{2}}}.$$

Example: Ramanujan's modular form, $\Delta(z)$

The Delta function

$$\Delta(q) = q \prod_{n \geq 1} (1 - q^n)^{24} \quad (q = e^{2\pi i z})$$
$$= q - 24q^2 + 252q^3 + \cdots$$

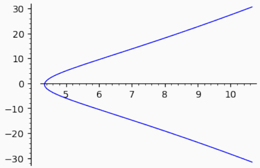
is a weight 12 modular form on $\Gamma = \mathrm{SL}(2, \mathbb{Z})$. This modular form was studied by Ramanujan. Its L-function is $L(s, \Delta) = 1 - 24/2^{s+5.5} + 252/3^{s+5.5} + \cdots$, and attempts to show that these coefficients are multiplicative led to the development of Hecke operators. The L-function satisfies the functional equation



$\Delta(z)$, visualized on the disk model of $\mathcal{H}$. In this representation, "six O'clock" is 0, the center is i, "noon" is $i\infty$.
Color represents argument, consecutive contours indicate doubled size.

$$\Lambda(s, f) := (2\pi)^{-s}\Gamma(s + \tfrac{11}{2})L(s, f) = \Lambda(1 - s, f).$$

Example: Elliptic Curve $Y^2 + Y = X^3 - X^2 - 10X - 20$



Consider the Elliptic curve $Y^2 + Y = X^3 - X^2 - 10X - 20$. Let $a(p) = (p+1) - \#E(\mathbb{F}_p)$ count deviation from the expected number of solutions on the curve over $\mathbb{F}_p$.

Then there is a weight 2 modular form on $\Gamma(11) \subset \mathrm{SL}(2, \mathbb{Z})$,

$$f(q) = q \prod_{n \geq 1} (1 - q^n)^2 (1 - q^{11n})^2,$$

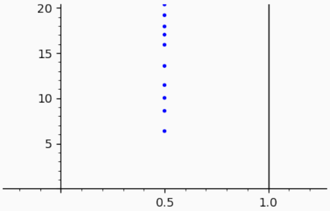
whose coefficients $a(p)$ match exactly the $a(p)$ defined above (an example of the Modularity theorem), and the L-functions associated to the curve and this modular form are the same:

$$L(s, E) = 1 - \frac{2}{2^{s+0.5}} - \frac{1}{3^{s+0.5}} + \cdots,$$

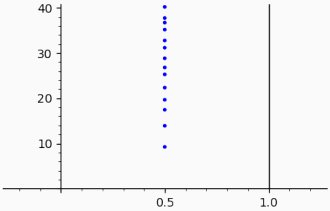
satisfying

$$\Lambda(s, E) := (22\pi)^{s/2} \Gamma(s + 1/2) L(s, E) = \Lambda(1 - s, E).$$

Both of these examples give Selberg L-functions. The analyticity and functional equation follow from the action of the matrix subgroup of $\mathrm{SL}(2, \mathbb{Z})$ on the modular form. The Euler product comes from the theory of Hecke operators. The Ramanujan conjecture $|a(n)| \ll n^{\epsilon}$ is the Hasse-Weil Bound on elliptic curves (for $L(s, E)$) or the highly nontrivial Deligne's Bound [Del71] (for general modular $L(s, f)$).



First zeros of $L(s, E)$



First zeros of $L(s, \Delta)$

A similar, but different, story

Typical L-functions

Half-integral weight modular forms

Computational Results and Methodology

No Euler products

Of the four requirements of the Selberg Class (analyticity, Ramanujan conjecture, a functional equation, and an Euler product), the most surprising to me is the Euler product. The other requirements all feel very "analytic", but the Euler product is feels fundamentally "arithmetic".

But it's known that a (nice) Euler product is essential to results like RH.

Davenport–Heilbronn series

For example, Davenport and Heilbronn [DH36] studied a Dirichlet series formed from a particular linear combination of Dirichlet L-functions,

$$L(s) = \frac{1 - i\theta}{2} L(s, \chi) + \frac{1 + i\theta}{2} L(s, \overline{\chi}),$$

where θ is a particular constant and $\chi = \chi_5(2, \cdot)$ is the unique primitive character mod 5 with $\chi(2) = i$. Then $L(s)$ satisfies the functional equation

$$\Lambda(s) := L(s)\Gamma(\tfrac{s+1}{2})(5/\pi)^{s/2} = \Lambda(1 - s),$$

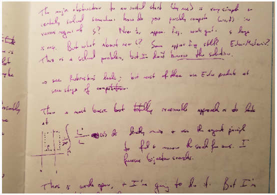
but has infinitely many zeros on the critical line and infinitely many zeros in the half-plane $\operatorname{Re} s > 1$.

The exceptional zeros appear to be sporadic: there are four zeros off the critical line with $0 < \operatorname{Im} s < 200$. Nonetheless, there are infinitely many.

Motivation

More generally, we expect that any Dirichlet series that satisfies the first three requirements of the Selberg class *but not an Euler product* should fail to satisfy a Riemann Hypothesis.

Until 2018, the only sort of example of this sort of not-quite-Selberg Dirichlet series and analysis I'd seen were formed from linear combinations of Selberg Class L-functions, like the Davenport–Heilbronn series.



But there is a class of Dirichlet series coming from half-integral weight modular forms, which (we think) aren't linear combinations of Selberg Class L-functions, and which don't have a multiplicative structure.

Half-integral weight modular forms

A modular form of half-integral weight k (so k here is in $\frac{1}{2}+\mathbb{Z}$) is a holomorphic function on $\mathcal{H}$ that transforms in a prescribed way under the action of a discrete subgroup $\Gamma \subseteq \mathrm{SL}(2,\mathbb{Z})$, satisfying

$$f(\gamma z) = j(\gamma, z)^k f(z)$$

for a half-integral factor of automorphy $j(\gamma, z)$. In the remainder of this talk, I'll consider the cocycle

$$j(\gamma, z) = \varepsilon_d^{-1}\left(\frac{c}{d}\right)\sqrt{cz+d}, \qquad \varepsilon_d = \begin{cases} 1 & d \equiv 1 \bmod 4, \\ i & d \equiv 3 \bmod 4. \end{cases}$$

Here, (c/d) is the Legendre symbol, and we will suppose that $\Gamma \subseteq \Gamma_0(4) = \{\left(\begin{smallmatrix} a & b \\ c & d \end{smallmatrix}\right) : b \equiv 0 \bmod 4\}$, so that we know that d is odd. Notice if you square $j(\gamma, z)$, it looks like a full-integral weight transformation law (possibly with a quadratic twist).

As with full-integer weight forms, we require that f be *holomorphic at all the cusps*, which implies that $f(z)$ can be written as a Fourier expansion

$$f(z) = \sum_{n \geq 0} a(n)e(nz).$$

If $a(0) = 0$ in all such Fourier expansions, then f is a half-integer weight cuspform.

There is a theory of Hecke operators, but it's a very different theory in comparison to the full-integer weight case. Hecke operators are indexed by square of primes $T(p^2)$. The action of these Hecke operators does not force the coefficients to be multiplicative. (They *do* relate the coefficients $a(np^2)$ and $a(n)$, but they do not relate coefficients at squarefree indices. Weird!). It is still true that there is a basis of forms that are eigenforms under (almost all) Hecke operators.

Shimura Correpondence

However, if $f = \sum_{n\geq 1} a(n)e(nz)$ is a half-integral weight $k > 1$ cuspform that is an eigenform of each Hecke operator $T(p^2)$, and if we denote the eigenvalues by $T(p^2)f = \alpha(p)f$, then we can define a sequence of coefficients $b(n)$ by

$$\sum_{n\geq 1} \frac{b(n)}{n^s} = \prod_p \left(1 - \frac{\alpha(p)}{p^s} + \frac{p^{2k-1}}{p^{2s}}\right)^{-1},$$

then

$$F(z) = \sum_{n\geq 1} b(n)e(nz)$$

is a full-integral weight $(2k-1)$ Hecke eigenform.

This is the Shimura Correspondence [Shi73]. Thus half-integral weight Hecke cuspforms don't have multiplicative coefficients or Euler products, but they correspond to full-integer weight cuspforms in the Selberg class.

The theta function

One example of a half-integral weight modular form is the theta function

$$\theta(z) = 1 + 2\sum_{n\geq 1} e^{2\pi i n^2 z},$$

which is a weight $1/2$ modular form on $\Gamma_0(4)$. This is a very natural object in the theory of Dirichlet series, as Riemann's first proof of the functional equation for $\zeta(s)$ uses this theta function in the form

$$\Theta(y) := \theta(iy/\sqrt{2}).$$

Riemann showed that

$$\pi^{-s/2}\Gamma(\tfrac{s}{2})\zeta(s) = \int_0^\infty \tfrac{1}{2}(\Theta(t) - 1)t^{s/2}\frac{dt}{t}$$

and derived the functional equation for $\zeta(s)$ from transformation laws for $\theta(z)$ (via Poisson summation). (A similar story is true for Dirichlet L-functions and twisted theta functions θ_χ).

Dirichlet series

Half-integral weight cusp forms of weight k on a matrix group Γ form a complex vector space $S_k(\Gamma)$. To any such cuspform $f(z) = \sum_{n \geq 1} a(n) e(nz)$, one can associate a Dirichlet series

$$L(s, f) = \sum_{n \geq 1} \frac{a(n)}{n^{s + \frac{k-1}{2}}},$$

but these Dirichlet series won't have Euler products, even if f is a Hecke eigenform.

Each such Dirichlet series have analytic continuation to $\mathbb{C}$ and satisfy a functional equation of the form

$$Q^s L(s, f) G(s) = \epsilon Q^{1-s} L(1-s, g) G(1-s),$$

where g is a modular form related to f via an involution of the form $g(z) \approx f(1/Nz)$. But in general (in contrast to the full-integral case), g is not a cusp form in the same space $S_k(\Gamma)$ — in general g can transform with a quadratically twisted factor of automorphy $\chi_N(\gamma) j(\gamma, z)^k$.

A priori, there are thus two differences between Dirichlet series coming from half-integral weight modular forms and the Selberg class: a typical half-integral weight modular form doesn't yield a symmetric functional equation, *and* the Dirichlet series won't have an Euler product.

However, for Hecke eigenforms on $\Gamma_0(4N)$, for N squarefree, it is possible to choose a related form with a symmetric functional equation.

Proposition (Hulse–Kıral–Lim–Lowry-Duda)

Let $f(z)$ be a Hecke eigenform of half-integral weight k on $\Gamma_0(4N)$ with (full-integer) weight $2k-1$ Shimura correspondent F. Then there is Hecke eigenform g of weight k on $\Gamma_0(16N^2)$ that also has Shimura correspondent F and whose Dirichlet series satisfies the symmetrical functional equation

$$\Lambda(s,g) = Q^s L(s,g) G(s) = \epsilon \Lambda(1-s,g)$$

for some $|\epsilon| = 1$.

(Aside: Frequently one can take g to be on $\Gamma_0(4N^2)$).

For the remainder of this talk, we consider only those half-integral weight k cuspidal Hecke eigenforms g that appear in the Proposition. Each such form has a Dirichlet series $L(s, g) = \sum_{n \geq 1} A(n) n^{-s}$ that has analytic continuation to $\mathbb{C}$ and a symmetric functional equation (Selberg class requirements 1 and 3).

Further, it is known [CN62] that

$$\sum_{n \leq X} |A(n)|^2 = c_g X,$$

so that the Ramanujan Conjecture $A(n) \ll n^{\epsilon}$ is true on average. (Heuristically it seems true).

What classical results are still true?

Such a Dirichlet series $L(s, g)$ is *very similar* to a Selberg Class L-function like $\zeta(s)$, and thus all proofs that work for the Selberg Class *but that completely avoid the Euler product* will apply. Not everything works: For example, to study $\zeta'(s)/\zeta(s)$ (as in the Prime number theorem), one method is to logarithmically differentiate the Euler product representation to get a well-behaved function in the region $\mathrm{Re}\, s > 1$ — but we can't do that here!

Nonetheless, one can prove the expected counting results.

Theorem

- $L(s, g)$ *has on the order of* $T \log T$ *nontrivial zeros with* $0 < \mathrm{Im}\, s < T$.
- $L(s, g)$ *has at most* $\log T$ *zeros (counting multiplicity) in any strip* $T < \mathrm{Im}\, s < T + 1$.

We can prove a few results that might look a bit odd in comparison with the Selberg Class, too.

Theorem

- *All nontrivial zeros of* $L(s, g)$ *are constrained to a strip* $1 - A < \operatorname{Re} s < A$. *(But typically* $A > 1$*).*
- *If* $L(s, g)$ *has at least one zero in the region* $\operatorname{Re} s > 1$, *then* $L(s, g)$ *has infinitely many, and there are* $\Omega(T)$ *in the region* $0 < \operatorname{Im} s < T$.

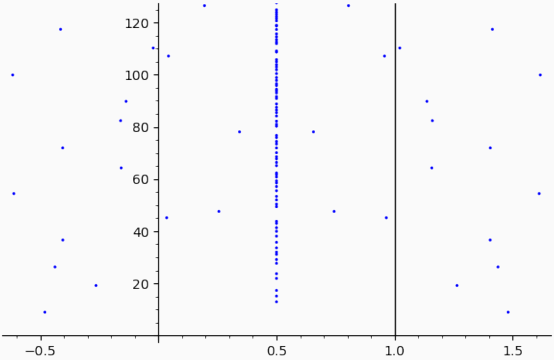
This last result follows from the general theory of almost periodic functions, but is somewhat uncommon now since Selberg Class L-functions don't have zeros in the domain of absolute convergence.

Fruits of our Labor

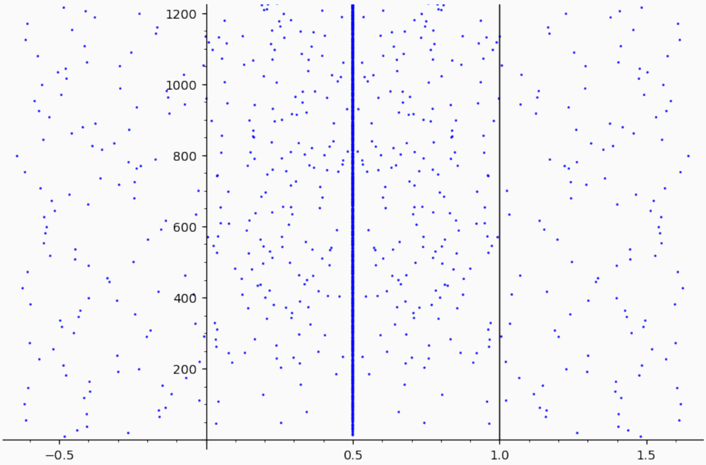
Typical L-functions

Half-integral weight modular forms

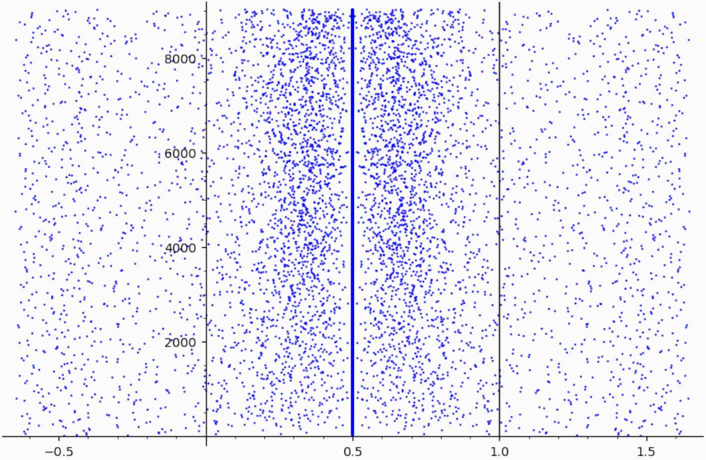
Computational Results and Methodology



These are zeros of the unique half-integral weight modular form g of weight $9/2$ on $\Gamma_0(4)$ (a form appearing in Shimura's paper [Shi73]). If $\eta(z) = e(z/24)\prod_{n\geq 1}(1 - e(nz))$ is the Dedekind η function (a 24th root of $\Delta(z)$), then this form is $g(z) = \eta(2z)^{12}\theta(z)^{-3}$.



Yoshida [Yos95] computed the first couple dozen of these zeros in 1995.



About 70 percent of the zeros in this image are on the critical line.

In order to compute with half-integral weight Dirichlet series, it is first necessary to compute the Fourier coefficients of the desired forms.

We use `Magma` to compute the Fourier expansions for a basis of forms for a vector space $S_k(\Gamma)$. (Magma uses an implementation of an algorithm from a Basmaji's PhD thesis [Bas96], which multiplies several full-integer weight forms by a variety of theta functions).

We then diagonalize this space with respect to the Hecke operators in `sagemath` to get a basis of Hecke eigenforms.

For a desired form, we symmetrize it as in our Proposition noted above. This was enough to compute the first hundred thousand Fourier coefficients of the weight $9/2$ form on $\Gamma_0(4)$.

With the Fourier coefficients, we compute values of $L(s, g)$ using the approximate functional equation. For the weight 9/2 form, this looks like

$$\Lambda(s, g) = \pi^{-s} \sum_{n \geq 1} \frac{a(n)}{n^s} V_1(n, s) + \pi^{s-1} \sum_{n \geq 1} \frac{a(n)}{n^{1-s}} V_2(n, 1-s)$$

where V_1 and V_2 are rapidly decaying Mellin transforms of Gamma functions.

In practice, we used a C++ implementation for symmetric degree 2 L-functions written by Rubinstein, called `lcalc`, and checked against the heuristic evaluation techniques of Yoshida [Yos95]. (A patched version of `lcalc` is included in `sagemath`).

To find the zeros themselves, we use a triple of techniques.

1. Zeros on the critical line
2. Quick heuristic methods for zeros off the critical line
3. Verification and checking for zeros off the critical line

Zeros on the critical line

If $\epsilon_1^2\epsilon = 1$ (where ϵ here is the sign of the functional equation), then $\epsilon_1\Lambda(s, g)$ is real-valued on the critical line. (In practice, we've only examined forms where $\epsilon = \pm 1$, so that $\Lambda(s, g)$ is either totally real or totally imaginary on the critical line).

Finding zeros on the critical line can be done pretty quickly by computing $\Lambda(s, g)$ at several points and looking for sign changes. These zeros are the easiest to compute.

Heuristic method for zeros off the critical line

To find zeros off the critical line, we've turned towards using Newton's Method of root finding (which works very well when it works, as $L(s, g)$ is complex analytic and all roots seem to be single roots).

That is, we compute several iterations of the map

$$s_n = s_{n-1} - \frac{L(s_{n-1}, g)}{L'(s_{n-1}, g)}$$

on a mesh of points. We ignore iterations that diverge and collect the various remaining candidate zeros for later verification.

Even though this is heuristic and in practice we re-find the same roots several times, this is our fastest technique in heuristic zero generation so far.

Numerical contour integration and the argument principle

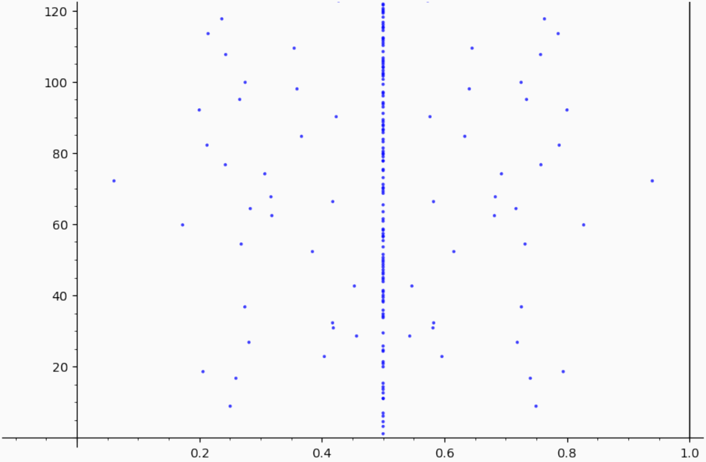
To verify counts and locations of zeros, we numerically compute integrals

$$\frac{1}{2\pi i}\int_C \frac{L'(z,g)}{L(z,g)}dz$$

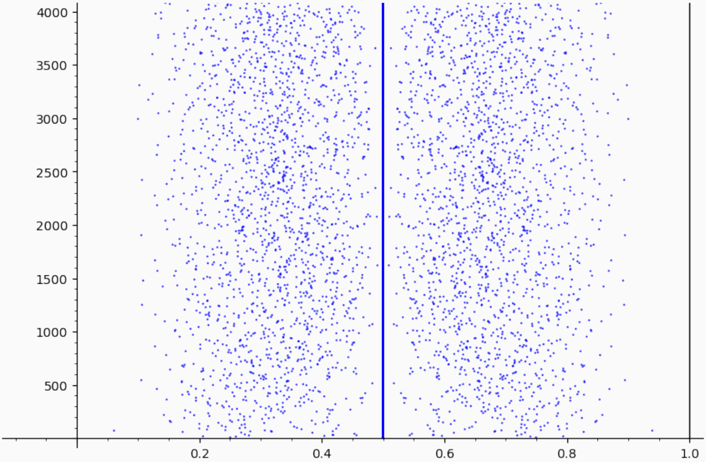
over contours C around heuristic zeros. By the argument principle, this integral gives the number of zeros (with multiplicity) inside the contour.

In comparison to Newton's method, this numerical integration is computationally intensive and slow. We're still working out the optimal way to heuristic and verifiable computation. But we believe we've found at least 99 percent of the first 150000 zeros for the weight 9/2 form indicated earlier.

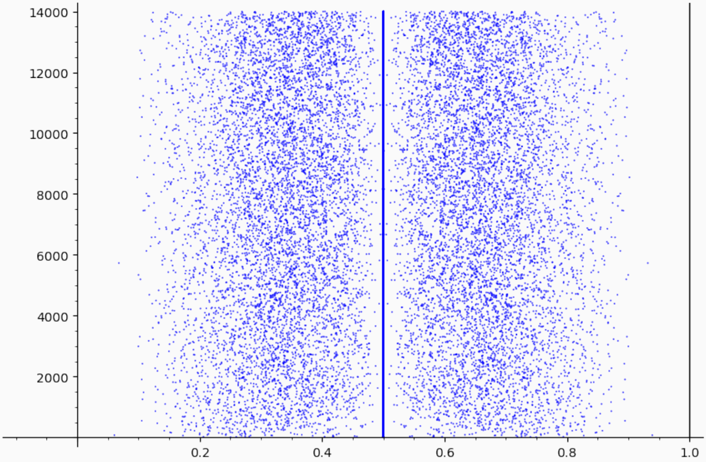
We've done this with other half-integral weight modular forms as well.



A weight 9/2 form on $\Gamma_0(12)$.



There don't seem to be any zeros outsize of the critical strip.



Approximately 65 percent of these zeros are on the critical line.

Pair Correlation

We can investigate statistics concerning the zeros as well. One nontrivial statistic is the pair correlation. For Selberg L-functions, the pair correlation is defined in terms of the spacing between the nontrivial zeros, weighted so that the expected spacing is 1 on average. Here, as we have lots of "exceptional" zeros, it's not clear what the right analogue is.

We investigated the pair correlation between the imaginary parts of zeros, normalized so that the typical spacing is 1 on average. That is, if $\rho_n = \sigma_n + i\gamma_n$ is the nth zero, then we consider spacings

$$\delta_n = c(\gamma_{n+1} - \gamma_n) \log c' \gamma_n,$$

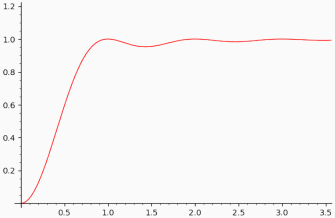
where c and c' come from the zero count $N(T)$ of zeros up to height T.

Then the pair correlation function is the distribution $\phi(u)$ such that as $M, N \to \infty$,

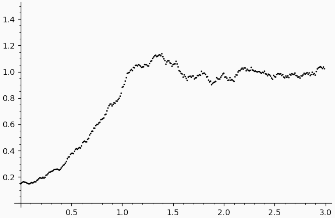
$$\frac{1}{M} \Big\{ (n, k) : N \leq n \leq N + M, k \geq 0, \delta_n + \cdots + \delta_{n+k} \in [\alpha, \beta] \Big\} \sim \int_\alpha^\beta \phi(t) dt,$$

(if this function exists).

The Montgomery Pair Correlation Conjecture posits that the pair correlation function for $\zeta(s)$ is $1 - \left(\frac{\sin(\pi x)}{\pi x}\right)^2$.

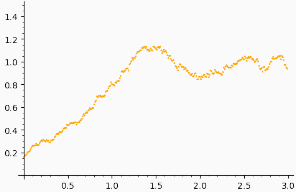


Computationally, the pair correlation function for the (normalized differences between imaginary parts of the) zeros of the weight 9/2 form on $\Gamma_0(4)$ look like the figure at right.

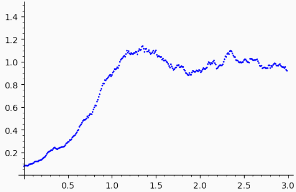


Qualitatively, these look similar. There is a similar repulsion phenomenon initially, and the shape is roughly similar. But they're also clearly not the same.

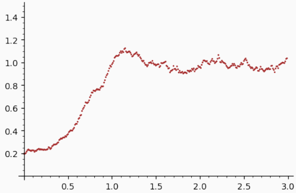
Let's examine estimated pair correlation functions for other forms.



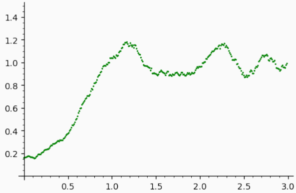
75k zeros of a weight $13/2$ form on $\Gamma_0(4)$



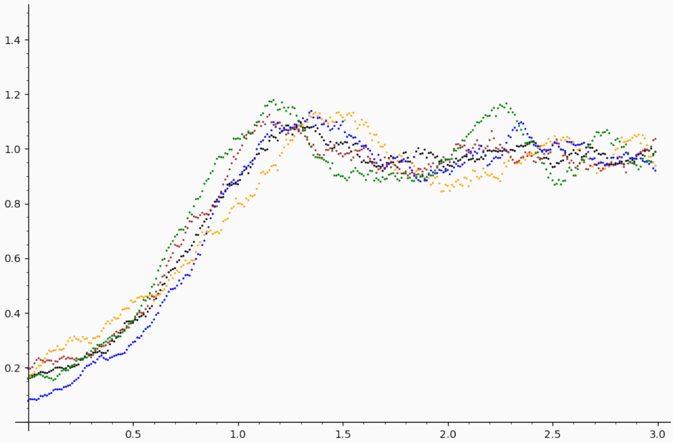
40k zeros of a weight $9/2$ form on $\Gamma_0(12)$



70k zeros of a weight $15/2$ form on $\Gamma_0(4)$



10k zeros of another weight $9/2$ form on $\Gamma_0(12)$

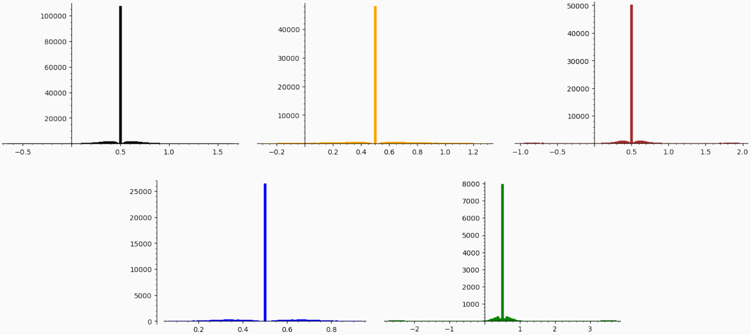


All five computed pair correlation approximations, plotted together. Notice how structurally similar they are, despite coming from different modular forms and over different ranges of zeros.

We don't know how to explain this.

We don't quite know where we're going, but what started as a purely exploratory investigation into a niche between linear combinations of L-functions and the Selberg class has transformed into an interesting little chestnut.

To end, I'll put (color coded) histograms of the real parts of the zeros we've computed for these five forms.



Thank you very much.

Please note that these slides (and references for the cited works) are (or will soon be) available on my website (davidlowryduda.com).

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