

Isaac Newton Institute for Mathematical Sciences
RMAw02 - Recent Perspectives in Random Matrix Theory and Number Theory

Computational methods for L-functions II
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Even Maclaurin summation works
well for $\zeta(s)$ and also for Dirichlet
L functions $L(s, \chi)$ because the Dirichlet
coefficients are very simple

Not very efficient for $\zeta(s)$ # terms needed
 $O(1/s)$

Much better to use Riemann S_{α}
or smoothed variants

Riemann Siegel Formula

$$Z(t) = e^{i\omega t} \zeta\left(\frac{1}{2} + it\right)$$

$$e^{i\omega t} \left(\frac{\Gamma\left(\frac{1}{4} + \frac{it}{2}\right)}{\Gamma\left(\frac{1}{4} - \frac{it}{2}\right)} \right)^{\frac{1}{2}} \pi^{\frac{it}{2}}$$

$Z(t)$ is real

Riemann-Siegel

$$Z(t) = 2 \underbrace{\sum_{n \leq t} n^{-1/2} (\cos(\omega t) - t \log n)}_{\text{main sum}} + R(t)$$

$$R(t) = O(t)^{Nt} \sum_0^{Nt} \frac{c_r p}{a^r} \quad \text{a asymptotic series (Berry studied asymptotic of the } c_r \text{'s)}$$

$$a = \left(\frac{t}{2\pi}\right)^{1/2} \quad N \lfloor a \rfloor p \quad \xi a \xi$$

(Formula can be extended to $s \neq \frac{1}{2} + it$ see Odlyzko-Schönhage for summary references)

$$C_1(p) = \psi(p) \sim (2\pi p^2 p^{-1/2}) / \cos 2\pi p$$

$$C_2(p) = \frac{1}{9\pi^2} \psi^{(3)}(p)$$

$$C_3(p) = \frac{1}{1842\pi^4} \psi^{(6)}(p) + \frac{1}{64\pi^2} \psi^{(2)}(p)$$

$$C_4(p) = -\frac{1}{53084\pi^4} \psi^{(9)}(p) - \frac{1}{3840\pi^4} \psi^{(5)}(p) - \frac{1}{64\pi^2} \psi^{(3)}(p)$$

Riemann used saddle point method to obtain $C_j, j \leq 5$. Reason such nice formulae are possible using sharp cut off, that all the Dirichlet coefficients are. Riemann starts with a representation for $\zeta(s)$ that involves geometric series identity $1/x = \sum x^n$

↑
Dirichlet coefficients of ζ

For a general L function smoothing is better

Titchmarsh showed error $\leq \frac{3}{2} \left(\frac{t}{2\pi}\right)^{3/4}$

if $\frac{t}{2\pi} > 25$, and we take just the

C_0 term

Gabcke showed error $\leq 0.53t^{\frac{5}{8}}$

if $t > 200$ and we take just the C_0 and C_1 terms

Odlyzko & Schönhage developed an algorithm to compute the main sum for $T \leq t < T + T^{1/2}$ in $O(t)$ operations provided a precomputation involving $O(T^{1/2} \log T)$ operations and bits of storage are carried out beforehand. This algorithm established Odlyzko's main result for computations

Main Lesson

Sm th things are nice

Smoothing as a technique in analytic number theory is over 100 years old

de la Vallée Poussin's proof of the prime number theorem involved showing

$$\psi(x) - \sum_{n \leq x} (\psi(n) - n) \sim \int_0^x \psi(t) dt$$

is asymptotic to $x^2/2$

$$(\psi(x) \sim \frac{x^2}{2}) \leftrightarrow \psi(x) \sim x$$

$$2\pi i \int_{(c)} \frac{y^s ds}{s(s+1)} \begin{cases} y & y \geq 1 \\ 0 & y \leq 1 \end{cases} \quad c > 0$$

$$\frac{\psi(x)}{x} - \sum_{n \leq x} \left(\frac{n}{x} \right) \Lambda(n) \sim \frac{1}{2\pi i} \int_{(c)} \frac{x^s}{s(s+1)} \left(\frac{F(s)}{F(s)} \right) ds$$

↑
extra factor
gives convergent integrals
on the 1 line (away from 1)

70's-2000's Many authors have used Laurik's smoothed approximate functional equation, though with varying sophistication. Laurik's method for controlling cancellation is often overlooked (method: use a parameter to control cancellation. Lagarias-Odlyzko mention it in their 1979 Artin L-function paper. I use it extensively in my computations).

1982 Berry-Keating gave a different smoothed approximate functional equation (for $\zeta(s)$).

Let

$$L(s) = \sum_n \frac{b(n)}{s^n}$$

absolutely convergent in $\operatorname{Re} s > \sigma_1$
and et

$$\Lambda(s) = O^s \prod_{j=1}^a M(\alpha_j s + \beta_j) L(s)$$

$$\alpha_j \in \mathbb{R}^+$$

$$\operatorname{Re} \beta_j \geq 0$$

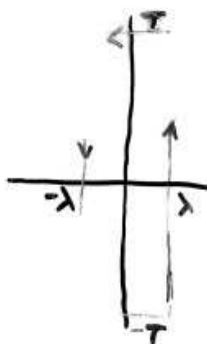
Assume that

- 1) $\Lambda(s)$ has meromorphic continuation to a l.o.f \mathbb{C} with simple poles at $s = s_j$ and corresponding residues r_j
- 2) $\Lambda(s) = w \overline{\Lambda(1-\bar{s})}$ for some $w \in \mathbb{C}$ $w \neq 0$
- 3) for any $c < d$ $\exists A_{c,d} > 0$ such that
$$L(\sigma + it) = O(t^A) \quad (c \leq \sigma \leq d)$$

Consider

$$2\pi i \int_C \frac{\Lambda(z+s)g(z+s)}{z} dz$$

where



$g(z)$ is entire and satisfies
for s fixed and $\lambda < \operatorname{Re} z \leq \lambda$,

$$\left| \frac{\Lambda(z+s)g(z+s)}{z} \right| \rightarrow 0 \text{ as } \operatorname{Im} z \rightarrow \infty$$

λ and T are chosen big enough
that all the poles s_1, s_2 are contained
in the rectangle, and also $\lambda > \sigma + \operatorname{Re} s$
and $\lambda > \sigma + \operatorname{Re} s - 1$

On the one hand we get

$$\Lambda(s)g(s) + \sum_{k=1}^l \frac{r_k g(s_k)}{s_k - s}$$

Now, as $T \rightarrow \infty$, \int_{C_2} and $\int_{C_4} \rightarrow 0$

On C use the Dirichlet series for $\Lambda(z+s)$ and change order of summation and integration

On C_3 apply the functional equation and then the Dirichlet series

By Stirling's formula

$$|\Gamma(s)| \sim (2\pi)^{\frac{1}{2}} |s|^{\sigma-\frac{1}{2}} e^{-|t|\frac{\pi}{2}}, \text{ as } |t| \rightarrow \infty$$

So that $|\Lambda(s)|$ decreases exponentially fast as $|t| \rightarrow \infty$. On the other hand, with $g(z) = 1$, we can show that $f_1(s, n)$ and $f_2(1-s, n)$ start off comparatively large (even though they decrease exponentially fast in n).

So a lot of cancellation must occur!

The "standard" trick is to choose

$$g(z) = \delta^{-z}$$

with $|\delta| = 1$ and chosen to cancel out most of the exponentially small size of the Γ factors.

With $g(z) = \delta^{-z}$ we can write $f_1(s, n)$ and $f_2(1-s, n)$ explicitly as incomplete integrals involving (unpleasant) special functions.

For example, when $a=1$ we have

$$\frac{\Gamma(v+u)}{u} = \int_0^{\infty} \Gamma(v,t) t^{u-1} dt, \quad \begin{array}{l} \operatorname{Re} u > 0 \\ \operatorname{Re}(v+u) > 0 \end{array}$$

where

$$\Gamma(v,t) = \int_t^{\infty} e^{-x} x^{v-1} dx$$

is the incomplete gamma function. So, by Mellin inversion (with $g(z) = \delta^{-z}$)

$$f_1(s,n) = \delta^{-s} \Gamma(\alpha s + \beta, (n\delta/Q)^{\frac{1}{\alpha}})$$

$$f_2(1-s,n) = \delta^{-s} \Gamma(\alpha(1-s) + \beta, (n\delta/Q)^{\frac{1}{\alpha}})$$

ex 1

$$\pi^{s/2} \Gamma\left(\frac{s}{2}\right) \zeta(s) \delta^s$$

$$\sum_1^{\infty} G\left(\frac{s}{2}, \pi n^2 \delta^2\right)$$

$$+ \delta \sum_n^{\infty} G\left(\frac{s}{2}, \pi n^2 \delta^{2-2}\right)$$

from pole at 0

$$s - \delta$$

from pole at s

$$G(z, w) = w^z \Gamma(z) \int_0^{\infty} e^{-wx} x^z dx \quad \text{Re } w > 0$$

ex 2 Dirichlet L f ctions

χ primitive conductor g

$\chi(x)$

$$\left(\frac{g}{\pi}\right)^{s/2} \Gamma\left(\frac{s}{2}\right) L(s, \chi) \delta^s$$

$$= \sum_1^{\infty} \chi(n) G\left(\frac{s}{2}, \pi n^2 \delta^2 / g\right)$$

$$+ \frac{\tau(\chi)}{\delta g^{s/2}} \sum_1^{\infty} \chi(n) G\left(\frac{1-s}{2}, \frac{\pi n^2}{\delta^2 g}\right)$$

$$\tau(\chi) = \sum_1^g \chi(m) e^{2\pi i m/g}$$

Notice an example if it takes

$$\frac{1}{2} \Gamma\left(\frac{s}{2}\right) \zeta(s)$$

$$s \quad s + \pi = \sum_{n=1}^{\infty} G\left(\frac{s}{2}, \pi n\right) + \pi \frac{(1-s)}{2} \sum_{n=1}^{\infty} G\left(\frac{1-s}{2}, \pi n\right)$$

$$- - s \quad s + \int_0^{\infty} \left(x^{\frac{s}{2}-1} + x^{-s} \right) \psi(x) dx$$

where

$$\psi(x) = \sum_{n=1}^{\infty} e^{-\pi n^2 x}$$

This is the expression Riemann discovered in his proof of the functional equation.

To control decay of $\Gamma\left(\frac{s}{2}\right)$ we can take for $s = \sigma + it$ with $t > 0$ $g(s) \delta^s$

$$\delta \begin{cases} t < 2c/\pi \\ e^{c\left(\frac{\pi}{2} - \frac{c}{t}\right) \frac{1}{2}} & t > 2c/\pi \end{cases}$$

f. to $c > 1$ for example larger c means faster convergence but also a proportional loss in accuracy.

$$G(z, w) \sim \frac{e^{\operatorname{Re} w}}{\operatorname{Re}(w - z)} \quad \text{if } \operatorname{Re}(w - z) > 0$$

we get exponential drop off roughly when

$$\operatorname{Re}(\pi n^2 \delta^2) \gg$$

$$\text{But } \operatorname{Re}(\pi n^2 \delta^2) = \pi n^2 \operatorname{Re} \delta^2 = \pi n^2 \frac{t}{c}$$

so terms starts to decay exponentially fast once

$$n \gg \sqrt{\frac{t}{\pi c}}$$

constant is #digits log 10

using properties of the incomplete gamma function one can relate

our

$$\pi^{-\frac{s}{2}} \Gamma\left(\frac{s}{2}\right) \zeta(s) \delta^s$$

as a main sum $\sum_{n=1}^N \frac{1}{n^s} + \frac{\chi(s)}{n^{1-s}} + \text{Remainder}$

with $N \sim \sqrt{\frac{t}{\pi c}}$ and most of the computation spent

Properties of the incomplete gamma function

$$\Gamma(z, w) = \int_w^{\infty} e^{-t} t^{z-1} dt \quad \arg z < \pi$$

$$\gamma(z, w) = \int_0^w e^{-t} t^{z-1} dt, \quad \arg z < \pi, \quad \operatorname{Re} w > 0$$

$$\Gamma(z, w) + \gamma(z, w) = \Gamma(z)$$

$$\gamma^*(z, w) = w^{-z} \gamma(z, w) \text{ is entire in } z \text{ and a } \Gamma(z)$$

As before let

$$G(z, w) = w^{-z} \Gamma(z, w)$$

$$g(z, w) = w^{-z} \gamma(z, w)$$

Integrate by parts

$$g(z, w) = e^{-w} \sum_0^{\infty} \frac{w^j}{(z)_j+1}$$

$$(z)_j = z(z+1)\dots(z+j-1) \quad f_j > 0$$

Converges nicely say $f_j \text{Re } z > 0$
when $w \ll z$

Another series, useful for $w \ll z$

$$g(z, w) = \sum_0^{\infty} \frac{(-1)^n}{n!} \frac{w^n}{z+n}$$

(not useful as w grows for the same reason
that $e^x = \sum \frac{e^x}{n!}$ is not useful for x is big)

Continued fraction

$$g(z, w) = \frac{e^{-w}}{z - \frac{z w}{z+1 - \frac{w}{z+2 - \frac{(z+1) \cdot w}{z+3 - \frac{2 \cdot w}{z+4 - (z+2)w}}}}}$$

works
well for $w \ll z$

Re a $g(z, w) = \underbrace{w^z \prod z}_{\text{leads to a main term}} - w G(z, w)$

For example for $\zeta(s)$,

$|w| < |z|$ is the region in the

first $G \frac{1}{2} \pi n^2 \delta^2$ sum

$$|\pi n^2 \delta| < \left| \frac{s}{2} \right| \quad \text{e } n < \left| \frac{s}{2\pi} \right|^{1/2}$$

and in the second $G \left(-\frac{s}{2} \frac{\pi n^2}{\delta^2} \right)$ sum

$$\left| \frac{\pi n^2}{\delta^2} \right| < \left| \frac{1-s}{2} \right|$$

$$\text{e } n < \left| \frac{1-s}{2\pi} \right|^{1/2}$$

$s = 1/2 + it$ gives a main sum consisting of approx $\frac{t}{2\pi}^{1/2}$ terms same as for Riemann Siegel formula

Integrate $G(z, w)$ by parts asymptotic series

$$G(z, w) = e^w \sum_0^M \frac{(1-z)^j}{(w)^j} + E_M(z, w)$$

$$E_M(z, w) = (1-z)^M G(z, M)$$

works for $w \gg z$

In that region the following continued fraction works

$$G(z, w) = \frac{e^w}{w + \frac{z}{w + \frac{z}{1 + \frac{2z}{w + \frac{3z}{1 + \frac{3z}{w + \dots}}}}}} \quad \text{asy. CT}$$

Intermediate region $z \sim w$
 is harder I that region $\Gamma(zw)$
 undergoes a transition

One can use Nielsens expansion to
 step through this region

$$\gamma(zw+d) \approx \gamma(zw) + w^2 e^{-\sum_{j=0}^A \frac{(1-E_j)}{(w)^j} (-e^{-d} e_j^d)} \left(-e^{-d} e_j^d \right)$$

$$e_j^d = \sum_{m=0}^j \frac{d^m}{m!}$$

|d| < |z|w

This is very well suited for example
 for L functions associated to modular forms
 since then we increment in eq step

Numerically unstable if d is big
 Overcome this by taking many smaller steps
 Not so well suited for degree L functions

One can also use Poisson summation method to handle $G(z, \omega)$ in the transition zone (soon)

or Temmes unform asy plots for $\sqrt{z} \omega$

$$Q(z, \omega) \sim \frac{\Gamma(z, \omega)}{\Gamma(z)}$$

$$\frac{1}{2} \operatorname{erfc}(\eta \sqrt{z/2}) + R_z(\eta)$$

$$\operatorname{erfc}(z) = \frac{2}{\sqrt{\pi}} \int_z^{\infty} e^{-t^2} dt$$

$$\lambda = \frac{\omega}{z} \quad \frac{1}{2} \eta^2 \quad \lambda \quad \log \lambda$$

sign η is chosen to be + for $\lambda >$

$$R_z(\eta) = \frac{e^{-z\eta^2}}{\sqrt{2\pi z}} S_z(\eta)$$

$$S_z(\eta) \sim \sum_{n=0}^{\infty} \frac{C_n(\eta)}{z^n} \quad \text{as } z \rightarrow \infty$$

$$C_0(\eta) = \frac{1}{\lambda-1} \eta \quad \left(\text{removable singularity at } \eta=0 (\lambda=1, z=a) \right)$$

$$C_1(\eta) = \eta^3 \quad \lambda^{-3} (\lambda-1)^2 z(\lambda)$$

$$\eta C_n(\eta) = \frac{d}{d\eta} C_n(\eta) + \frac{\eta}{\lambda} \gamma_n \quad n \geq 1$$

where

$$\Gamma^*(z) \sim \sum_0^{\infty} \frac{c^n \gamma_n}{z^n}$$

$$\Gamma^*(z) = \sqrt{\frac{z}{2\pi}} e^z z^{-z} \Gamma(z)$$

$$\gamma_0 = 1 \quad \gamma_1 = 12 \quad \gamma_2 = 288 \quad \gamma_3 = 51840$$

When $a > 1$ we get much more painful incomplete integrals.

For example, if $\alpha_1 = \dots = \alpha_a = 1/2$

$$f_1(s, n) = \delta^{-s} \int_{(n\delta/a)^2}^{\infty} E_{\alpha}(t) t^{\frac{s}{2} + \mu - 1} dt$$

$$f_2(1-s, n) = \delta^{-s} \int_{(n\delta/a)^2}^{\infty} E_{\alpha}(t) t^{\frac{1-s}{2} + \mu - 1} dt$$

where

$$\mu = \frac{1}{2} \sum_1^a \beta_j$$

$$E_{\alpha}(w) = \int_0^{\infty} \dots \int_0^{\infty} \prod u_j^{\alpha_j - 1} e^{-w^{\frac{1}{\alpha}} (\frac{1}{u_1} + \frac{u_1}{u_2} + \dots + \frac{u_{a-2}}{u_{a-1}} + u_a)} \frac{du_1}{u_1} \dots \frac{du_{a-1}}{u_{a-1}}$$

(when $a=2$, $E_{\alpha}(w) = 2 K_{\alpha, -\alpha}(2w^{\frac{1}{\alpha}})$, i.e. we get incomplete integrals of the K-Bessel function)

Now \hat{h} is also rapidly decreasing \circ

$$\sum_{m \neq 0} \hat{h}\left(\frac{m}{\Delta}\right)$$

quickly becomes negligible as $\Delta \rightarrow 0$

So

$$\Delta \sum_{m=-\infty}^{\infty} h(\Delta m) \approx \hat{h}(0) \int_{-\infty}^{\infty} h(x) dx$$

i.e. the Riemann sum makes for a great approx

This approach completely avoids the need for computing special functions. The most complicated thing we need to evaluate is the gamma function

We also have more freedom in choosing $g(z)$ since we don't need to know much (for ex series expansions) about $f(s, n)$.

Rather than work with the incomplete integrals we work directly with

$$f_1(s, n) = \frac{1}{2\pi i} \int_{\gamma-i\infty}^{\gamma+i\infty} \prod_{j=1}^r \Gamma(\alpha_j(s+z) + \beta_j) \frac{g(s+z)}{z} \left(\frac{Q}{n}\right)^z dz$$

Ignoring the $g(s+z)$ for now, we note that the integrand is rapidly decreasing. It pays to be naive and compute the integral as a Riemann sum!

Rough idea Let $h: \mathbb{R} \rightarrow \mathbb{C}$ be smooth and rapidly decreasing. By Poisson summation

$$\Delta \sum_{m \in \mathbb{Z}} h(m\Delta) = \sum_{n \in \mathbb{Z}} \hat{h}\left(\frac{n}{\Delta}\right)$$

with

$$\hat{h}(u) = \int_{-\infty}^{\infty} h(x) e^{-2\pi i x u} dx$$

Substitute $z = v + iu$

$$f_1(s, n) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \prod \Gamma(\alpha_j(s+v+iu) + \beta_j) \frac{g(s+v+iu) (Q/n)^{v+iu}}{v+iu}$$

We thus find (rearrange sums too)

$$\Lambda(s)g(s) \approx \sum_1^J \frac{r_k g(s_k)}{s-s_k} + Q^{s+v} \frac{\Delta}{2\pi} \sum_{m_1=M}^M H_1(m_1) \sum_1^N \frac{b(n)}{n^{s+v+im_1}}$$

$$+ \omega Q^{1-s+v} \frac{\Delta}{2\pi} \sum_{m_2=M}^M H_2(m_2) \sum_1^N \frac{\bar{b}(n)}{n^{1-s+v+im_2}}$$

where

$$H_1(u) = \prod \Gamma(\alpha_j(s+v+iu) + \beta_j) \frac{g(s+v+iu)}{v+iu} Q^{iu}$$

$$H_2(u) = \prod (\alpha_j(1-s+v+iu) + \bar{\beta}_j) \frac{g(s-v+iu)}{v+iu} Q^{iu}$$

So, we compute $\Lambda(s)$ from the values of the Dirichlet series evaluated at equally spaced points to the right of s and $1-s$

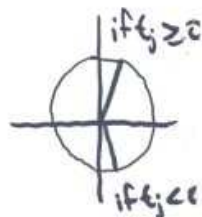
Choice of g

Let

$$t_j = \text{Im}(\alpha_j s + \beta_j)$$

$$\delta_j = \exp(i \text{sgn}(t_j) (\frac{\pi}{2} - \phi_j))$$

$$\phi_j = \begin{cases} \pi/2 & \text{if } |t_j| \leq 2c/\pi \\ \frac{c}{|t_j|} & \text{if } |t_j| > 2c/\pi \end{cases}$$



$c > 0$ is a free parameter. Larger c means faster conv. but more loss of precision.

Set

$$g(w) = \exp(A(w-s)^2) \prod_{j \in i} \delta_j^{-\alpha_j w + \beta_j}$$

allows us to cut down on the domain of integration.

A can't be large though, since we need the Fourier transform of this factor to have small support.

controls the

$$\prod \Gamma(\alpha_j s + \beta_j)$$

$$A = \frac{1}{16\pi^2 \log 10} \frac{1}{\text{Digits}}$$

$$\Delta = \frac{2\pi}{\log 10} \frac{v}{\text{Digits}}, \quad v \text{ is a free parameter}$$

If it is too large or too small we lose precision
(with $v=1.6$, $\text{Digits}=12$, we have $\Delta = .136$)

$$M = \frac{2 \log^2(10) \text{Digits}^2}{v}$$

$$N = O\left(Q(1+1)^{\sum \chi_j}\right)$$

↑
the Q that appears in the functional equation: For $L(s, \chi)$, $Q = \left(\frac{q}{\pi}\right)^{1/2}$, q conductor of χ