PAIR CORRELATION CONJECTURE

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Contents

1. Introduction

Montgomery introduces the function $F(\alpha)$ defined as

$$F(\alpha) = F(\alpha, T) = \left(\frac{T}{2\pi}\log T\right)^{-1} \sum_{0<\gamma,\gamma'\leqslant T} T^{i\alpha(\gamma-\gamma')} w(\gamma-\gamma'),$$

where α and $T \geqslant 2$ are both real and $w(u) = 4/(4+u^2)$. It can be readily observed that F is real-valued as $F(\alpha) = \overline{F(\alpha)}$ and F is even; $F(\alpha) = F(-\alpha)$. It is however not immediately obvious that $F(\alpha) \geqslant 0$. In the statement of main theorem in his paper, Montgomery states that if $T > T_0(\epsilon)$, then $F(\alpha) \geqslant -\epsilon$ for all α, which is a weaker statement.

The idea behind the proof of nonnegativity of $F(\alpha)$ is that we can decouple the term $w(\gamma-\gamma')$ not as a product $g(\gamma)g(\gamma')$ but as an improper integral $\int_{-\infty}^{\infty} g(\gamma, x)g(\gamma', x)\,dx$.

We consider the improper integral

$$\int_{-\infty}^{\infty} \frac{dx}{(1+(x-a)^2)(1+(x-b)^2)}.$$

Let

$$f(z) = \frac{1}{(1+(z-a)^2)(1+(z-b)^2)}.$$

Let $R > 0$. We take γ_R be the line segment from $-R$ to R and Γ_R to be the semicircle of radius R in positive orientation, i.e., $\Gamma_R(t) = Re^{it}$ with $t \in [0, \pi]$. Then by Cauchy's residue theorem we have

$$\int_{\gamma_R+\Gamma_R} f(z)\,dz = 2\pi i(\mathrm{Res}(f, a+i) + \mathrm{Res}(f, b+i)).$$

It can be easily seen that the integral of f over Γ_R goes to 0 as $R \to \infty$ due to the following estimate

$$\left|\int_{\Gamma_R} f(z)\,dz\right| \leqslant \frac{\pi R}{((R-a)^2-1)((R-b)^2-1)}.$$

Hence we have

$$\int_{-\infty}^{\infty} f(x)\,dx = \lim_{R\to\infty}\int_{\gamma_R+\Gamma_R} f(z)\,dz = 2\pi i(\mathrm{Res}(f, a+i) + \mathrm{Res}(f, b+i)).$$

Now observe that

$$\begin{aligned}\operatorname{Res}(f, a+i) &= \lim_{z\to a+i}(z-a-i)f(z)\\ &= \lim_{z\to a+i}\frac{1}{(z-a+i)(z-b-i)(z-b+i)}\\ &= \frac{1}{2i(a-b)(a-b+2i)}.\end{aligned}$$

Similarly, we have

$$\operatorname{Res}(f, b+i) = \frac{1}{2i(b-a)(b-a+2i)} = \frac{1}{2i(a-b)(a-b-2i)}.$$

Thus we have

$$\operatorname{Res}(f, a+i) + \operatorname{Res}(f, b+i) = \frac{1}{i(4+(a-b)^2)}$$

and the integral evaluates to

$$\int_{-\infty}^{\infty}\frac{dx}{(1+(x-a)^2)(1+(x-b)^2)} = \frac{2\pi}{4+(a-b)^2} = \frac{\pi}{2}w(a-b).$$

We can write

$$\left(\frac{T}{2\pi}\log T\right)F(\alpha) = \frac{2}{\pi}\sum_{0<\gamma,\gamma'\leqslant T}T^{i\alpha(\gamma-\gamma')}\int_{-\infty}^{\infty}\frac{dx}{(1+(x-\gamma)^2)(1+(x-\gamma')^2)}.$$

Since we have a finite sum we can interchange the integral and sum to obtain

$$\begin{aligned}\left(\frac{T}{2\pi}\log T\right)F(\alpha) &= \frac{2}{\pi}\int_{-\infty}^{\infty}\sum_{0<\gamma,\gamma'\leqslant T}\frac{T^{i\alpha(\gamma-\gamma')}}{(1+(x-\gamma)^2)(1+(x-\gamma')^2)}\\ &= \frac{2}{\pi}\int_{-\infty}^{\infty}\left|\sum_{0<\gamma\leqslant T}\frac{T^{i\alpha\gamma}}{1+(x-\gamma)^2}\right|^2 dx.\end{aligned}$$

The Montgomery's function $F(\alpha)$ should be thought of as a family of functions parametrized by T. We now state the main result of Montgomery concerning the behavior of $F(\alpha)$ in the unit interval.

THEOREM 1.1. *Assume RH to be true. Then for every fixed* $0\leqslant\alpha<1$ *we have*

$$F(\alpha) = (1+o(1))T^{-2\alpha}\log T + \alpha + o(1) \tag{1.1}$$

as $T\to\infty$. *This estimate holds uniformly for* $0\leqslant\alpha\leqslant 1-\epsilon$.

Later Montgomery along with Goldston showed that the estimate (1.1) holds uniformly for $0\leqslant\alpha\leqslant 1$.

Note that the function $T^{-2|\alpha|}\log T$ behaves in the limit as a Dirac δ-function as $T^{-2|\alpha|}\log T\to 0$ as $T\to\infty$ for every $\alpha\neq 0$ and

$$\int_{-A}^{A}T^{-2|\alpha|}\log T\,d\alpha = 2\int_0^A T^{-2\alpha}\log T\,d\alpha = \big[-T^{-2\alpha}\big]_0^A = 1-T^{-2A}$$

tends to 1 as $A\to\infty$.

Montgomery starts off proving Theorem 1.1 by working with the following explicit formula

$$\sum_{n\leqslant x}\frac{\Lambda(n)}{n^s} = \frac{x^{1-s}}{1-s} - \frac{\zeta'}{\zeta}(s) - \sum_{\rho}\frac{x^{\rho-s}}{\rho-s} + \sum_{n=1}^{\infty}\frac{x^{-2n-s}}{2n+s},$$

where $s \neq 1, s \neq \rho, s \neq 2n$ and the term $n = x$ is counted with weight $1/2$ if x is a prime power (see Exercise 4 on page 408 of Montgomery and Vaughan). If we assume RH and plug in $s = \sigma + it$ and $\rho = 1/2 + i\gamma$ we obtain

$$\sum_{n \leqslant x} \frac{\Lambda(n)}{n^{\sigma+it}} = \frac{x^{1-\sigma-it}}{1-\sigma-it} - \frac{\zeta'}{\zeta}(\sigma+it) - \sum_{\gamma} \frac{x^{1/2+i\gamma-\sigma-it}}{1/2+i\gamma-\sigma-it} + \sum_{n=1}^{\infty} \frac{x^{-2n-\sigma-it}}{2n+\sigma+it}.$$

Rearranging the terms we get
(1.2)

$$\sum_{\gamma} \frac{x^{i\gamma-it}}{\sigma-1/2+it-i\gamma} = x^{\sigma-1/2}\left(\frac{\zeta'}{\zeta}(\sigma+it) - \frac{x^{1-\sigma-it}}{1-\sigma-it} + \sum_{n \leqslant x} \frac{\Lambda(n)}{n^{\sigma+it}} - \sum_{n=1}^{\infty} \frac{x^{-2n-\sigma-it}}{2n+\sigma+it}\right).$$

Reflecting σ along the critical line, i.e., replacing σ by $1-\sigma$ we get
(1.3)

$$\sum_{\gamma} \frac{x^{i\gamma-it}}{1/2-\sigma+it-i\gamma} = x^{1/2-\sigma}\left(\frac{\zeta'}{\zeta}(1-\sigma+it) - \frac{x^{\sigma-it}}{\sigma-it} + \sum_{n \leqslant x} \frac{\Lambda(n)}{n^{1-\sigma+it}} - \sum_{n=1}^{\infty} \frac{x^{-2n-1+\sigma-it}}{2n+1-\sigma+it}\right).$$

Subtracting the left hand side of (1.3) form (1.2) we end up with

$$(2\sigma-1)\sum_{\gamma} \frac{x^{i\gamma-it}}{(\sigma-1/2)^2+(t-\gamma)^2}$$

Using the identity

$$\frac{\zeta'}{\zeta}(s) = -\sum_{n=1}^{\infty} \frac{\Lambda(n)}{n^s}$$

for $\sigma > 1$ and subtracting the right hand side of (1.3) form (1.2) we get

$$\begin{aligned} x^{\sigma-1/2}\frac{\zeta'}{\zeta}(\sigma+it) - \frac{x^{1/2-it}}{1-\sigma-it} + x^{\sigma-1/2}\sum_{n \leqslant x} \frac{\Lambda(n)}{n^{\sigma+it}} - \sum_{n=1}^{\infty} \frac{x^{-2n-1/2-it}}{2n+\sigma+it} \\ - x^{1/2-\sigma}\frac{\zeta'}{\zeta}(1-\sigma+it) + \frac{x^{1/2-it}}{\sigma-it} - x^{1/2-\sigma}\sum_{n \leqslant x} \frac{\Lambda(n)}{n^{1-\sigma+it}} + \sum_{n=1}^{\infty} \frac{x^{-2n-1/2-it}}{2n+1-\sigma+it}. \end{aligned}$$

Simplifying it we get

$$\begin{aligned} -x^{\sigma-1/2}\sum_{n > x} \frac{\Lambda(n)}{n^{\sigma+it}} - \frac{(2\sigma-1)x^{1/2-it}}{(\sigma-it)(1-\sigma-it)} - x^{1/2-\sigma}\frac{\zeta'}{\zeta}(1-\sigma-it) - x^{1/2-\sigma}\sum_{n \leqslant x} \frac{\Lambda(n)}{n^{1-\sigma+it}} \\ - \sum_{n=1}^{\infty} \frac{(2\sigma-1)x^{-2n-1/2-it}}{(\sigma+it+2n)(\sigma-1-it-2n)} \end{aligned}$$

Equating the two we obtain

$$\begin{aligned} (2\sigma-1)\sum_{\gamma} \frac{x^{i\gamma-it}}{(\sigma-1/2)^2+(t-\gamma)^2} = & -x^{-1/2-it}\sum_{n \leqslant x} \Lambda(n)\left(\frac{x}{n}\right)^{1-\sigma+it} - x^{-1/2-it}\sum_{n > x} \Lambda(n)\left(\frac{x}{n}\right)^{\sigma+it} \\ & - x^{1/2-\sigma}\frac{\zeta'}{\zeta}(1-\sigma-it) - \frac{(2\sigma-1)x^{1/2-it}}{(\sigma-it)(1-\sigma-it)} \\ & - \sum_{n=1}^{\infty} \frac{(2\sigma-1)x^{-2n-1/2-it}}{(\sigma+it+2n)(\sigma-1-it-2n)} \end{aligned}$$

Multiplying by the factor x^{it} on both side we get

$$\begin{aligned}(2\sigma-1)\sum_{\gamma}\frac{x^{i\gamma}}{(\sigma-1/2)^2+(t-\gamma)^2} = &- x^{-1/2}\sum_{n\leqslant x}\Lambda(n)\left(\frac{x}{n}\right)^{1-\sigma+it} - x^{-1/2}\sum_{n>x}\Lambda(n)\left(\frac{x}{n}\right)^{\sigma+it}\\ &- x^{1/2-\sigma+it}\frac{\zeta'}{\zeta}(1-\sigma-it) - \frac{(2\sigma-1)x^{1/2}}{(\sigma-it)(1-\sigma-it)}\\ &- x^{-1/2}\sum_{n=1}^{\infty}\frac{(2\sigma-1)x^{-2n}}{(\sigma+it+2n)(\sigma-1-it-2n)}.\end{aligned}$$