NUMERICAL APPROXIMATION OF THE MASSER-GRAMAIN CONSTANT TO FOUR DECIMAL DIGITS: $\delta = 1.819...$

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Abstract. We prove that the constant δ studied by Masser, Gramain, and Weber, satisfies $1.819776 < \delta < 1.819833$, and disprove a conjecture of Gramain. This constant is a two-dimensional analogue of the Euler-Mascheroni constant; it is obtained by computing the radius r_k of the smallest disk of the plane containing k Gaussian integers. While we have used the original algorithm for smaller values of k, the bounds above come from methods we developed to obtain guaranteed enclosures for larger values of k.

1. Introduction

The Masser-Gramain constant δ is a two-dimensional generalization of the Euler-Mascheroni constant:

$$\delta = \lim_{n\to\infty}\left(\sum_{k=2}^{n}\frac{1}{\pi r_k^2} - \log n\right),$$

where r_k is the minimum radius of a closed disk containing at least k points with integer coordinates — we will say in the following "integer points" — where the center of the disk is not necessarily an integer point. Gramain and Weber showed in [5]:

$$1.811447299 < \delta < 1.897327117,$$

and Gramain conjectured that $\delta = 1 + 2\log\pi - \log 2 + 2\gamma - 2\log L$, where γ is Euler-Mascheroni's constant and $L = 2\int_0^1 \mathrm{d}x/\sqrt{1-x^4}$ is Gauss' lemniscate constant, which would give $\delta \approx 1.822825$ [4].

Using new theoretical results, new algorithms, and intensive computations, we improve the result of Gramain and Weber to

$$1.819776 < \delta < 1.819833,$$

which disproves Gramain's conjecture. We used an exact computation of r_k up to $k = 10^6 - 1$, using essentially the same algorithm as Gramain and Weber, but using a multi-core cluster during several weeks. For $10^6 \le k < 10^9$, we used the bisection algorithm described in §4, which gives for each value of k a tight interval enclosing r_k. Finally for $k \ge 10^9$ we used a new analytic lower bound on r_k described in §3, which is an original result by itself. In §2 we give an improved analytic lower bound on r_k, which was used in our computation only to initialize the bisection method from §4; however the way this lower bound is derived is original and might also be useful in other contexts. In their work, Gramain and Weber performed exact computations up to $k = 1400$ and then used analytic bounds on r_k.

The first values of the r_k sequence are $r_2 = 1/2$, $r_3 = r_4 = \sqrt{2}/2$, $r_5 = 1$, $r_6 = \sqrt{5}/2$, $r_7 = 5/4$, $r_8 = r_9 = \sqrt{2}$. Notice that, for those small values of k, the squared radius r_k^2 is rational; this is true for all values of k [5]. The classical way to get an enclosure for δ is first to get an enclosure for the partial sum $s_n := \sum_{k=2}^{n} 1/(\pi r_k^2)$, and then to use an analytic enclosure for the tail from $n+1$ to ∞. To get a tight analytic enclosure, we need tight upper and lower bounds for r_k. Gramain and Weber in [5] used a lower bound of Chaix for the radius r_k (to simplify, we use r instead of r_k whenever there is no ambiguity):

Lemma 1 (Chaix [2])**.** *For $k > 1.364 \cdot 10^7$, $k < \pi r^2 + 30.84274723\, r^{2/3}$.*

We will prove in §3 a tighter result:

Lemma 2. *For $r \geq 5$, we have $k < \pi r^2 + 7.213 r^{2/3} + 1.5 r^{1/2}$.*

For $k \geq 10^9$, which implies $r > 17841$ from Lemma 1, it follows $k < \pi r^2 + 7.507 r^{2/3}$.

There is a simple upper bound on the radius that is used in most proofs. This is the same property as Proposition 3 from [5]; the idea of its proof is reproduced here for completeness. Note that experiments from §4 have shown that this bound is hard to improve on.

Lemma 3. *For $k \geq 2$, we have $r < \sqrt{\frac{k-1}{\pi}}$.*

Proof. This is an immediate corollary of a theorem by Pólya and Szegö [8] that states that any compact domain of area A can be translated so that it contains $\lfloor A \rfloor + 1$ points. □

Once we have a partial sum s_n, the following main theorem makes use of the bounds from Lemmas 2 and 3 to produce an enclosure of δ.

Theorem 1. *Assume $k < \pi r^2 + \alpha r^{2/3}$ holds for $k \geq 10^9$ and some $\alpha < 30.85$. Then for $n \geq 10^9$, we have:*

$$s_n - \log n + \frac{1}{2n} < \delta < s_n - \log\left(n + \frac{1}{2}\right) + \frac{\beta}{n^{2/3}},$$

for any $\beta \geq 1.0242 \cdot \alpha$. In particular for $\alpha = 7.507$ (Lemma 2) we can take $\beta = 7.69$.

Proof. From the main theorem in [5]:

$$\delta > (s_n - \log n) + \lim_{N \to \infty} \left(\log \frac{n}{N+1} + \sum_{k=n}^{N} \frac{1}{k} \right).$$

Now consider n fixed, and let N tend to infinity. Let ψ be the digamma function, that is, the logarithmic derivative of the Γ function. Since the sum $\sum_{k=n}^{N} 1/k$ equals $\psi(N+1) - \psi(n)$, and $\lim_{N \to \infty} \psi(N+1) - \log(N+1) = 0$, we get $\delta \geq s_n - \psi(n)$. Since $\log n > \psi(n) + 1/(2n)$ for $n \geq 1$, this proves the lower bound.

From the hypothesis $k < \pi r^2 + \alpha r^{2/3}$, and $r < \sqrt{k/\pi}$ by Lemma 3, we deduce

$$\frac{1}{\pi r^2} < \frac{1}{k - \alpha (k/\pi)^{1/3}} = \frac{1}{k}\left(1 + \frac{\alpha}{k^{2/3}\pi^{1/3}}\left(1 - \frac{\alpha}{k^{2/3}\pi^{1/3}}\right)^{-1}\right) < \frac{1}{k} + \frac{2\beta}{3k^{5/3}}.$$

It follows for $N > n \geq 10^9$:

$$\begin{aligned} \delta &\leq s_n + \lim_{N \to \infty}\left(-\log N + \sum_{k=n+1}^{N} \frac{1}{k} + \frac{2\beta}{3k^{5/3}}\right) < s_n - \psi(n+1) + \int_n^{\infty} \frac{2\beta}{3k^{5/3}} \mathrm{d}k \\ &= s_n - \psi(n+1) + \frac{\beta}{n^{2/3}} < s_n - \log(n + 1/2) + \frac{\beta}{n^{2/3}}, \end{aligned}$$

since $\psi(n + 1/2) > \log n$ for $n \geq 1$. □

We describe in §3 how the analytic lower bound from Lemma 2 was obtained.

2. An improved analytic lower bound on r_k

2.1. **Relating disk radius and number of integer points.** Let us consider a disk of area πr^2 containing k integer points. The disk is first split into four quadrants according to the horizontal and vertical lines going through its center. The four quadrants and the integer points they contain[1] are then moved away. A cross of area $4r + 1$ is placed between them.

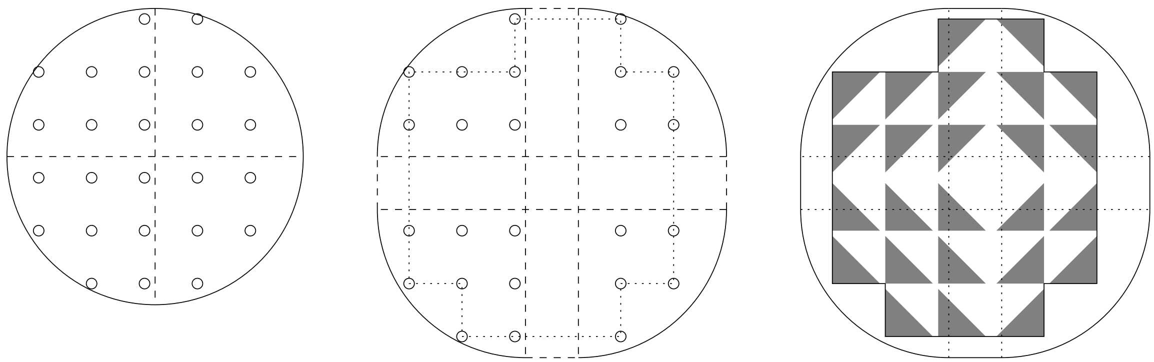

Figure 1. A disk of area πr^2 is first expanded by adding a cross of area $4r+1$. Then k unit squares are attached to the k integer points of the disk. The bijection between squares and integer points is represented by gray triangles showing which square corners are attached to which integer points.

Unit squares can now be embedded in the expanded disk and placed at integer coordinates. There are exactly k such squares. This is shown on Figure 1 by associating to each integer point a square. A point in the upper right quadrant gets the square whose upper right corner is at this integer point. The process is symmetric for the other quadrants. The added cross ensures that points near the horizontal and vertical diameters do not share squares.

Let T' be the area of the expanded disk that is not occupied by squares. The equality $\pi r^2 + 4r + 1 = k + T'$ holds. If we consider only the area T of the original disk which does not contain squares, we get the following relation instead, where $0 \le T' - T < 4$ corresponds to the area of the added cross which is not occupied by squares:

$$\pi r^2 + 4r + 1 \ge k + T.$$

2.2. **Bounding the disk border.** In Proposition 4 from [5], the authors consider convex curvilinear right-angled triangles of width 1 to obtain a lower bound on the area T. However, they use triangles of heights 1 and 2 only. Here, we consider simple right-angled triangles only, but of any height. The height might not even be an integer, as shown on Figure 2.

Lemma 4. *If a disk of radius r contains $k \ge 5$ integer points, then $k < \pi r^2 + 4r + 1 - T$ with*

$$T/4 \ge -2\sqrt{r-1} + r/\sqrt{2}.$$

[1] If an integer point is on the border between several quadrants, an arbitrary one is chosen as its container, for instance the rightmost and/or topmost one.

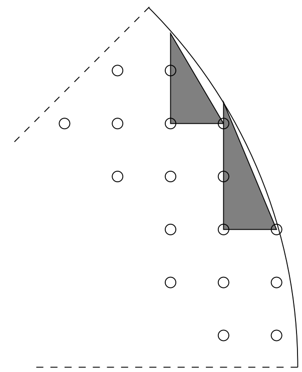

FIGURE 2. Filling the disk border of the first octant with right triangles of noninteger heights. In the proof of Lemma 4, the height of the triangles will not be that optimal.

Proof. Let $x + iy$ be the center of a disk of radius r. Let $(u_i)_{0\leq i\leq n}$ be a finite increasing sequence of real numbers with $u_0 \geq 1$. For $s \geq 1$, we define $\alpha_s := r \cos \arctan(1/s) = rs/\sqrt{s^2+1}$.

Between abscissas $\lceil x + \alpha_{u_i} \rceil$ and $\lceil x + \alpha_{u_{i+1}} \rceil$, triangles of height u_i can be used to fill the disk border. Indeed, by definition of α_s, at the right of $x + \alpha_s$, the tangent of the disk is of slope larger than s (in absolute value).

Similarly, between abscissas $\lceil x + \alpha_{u_n} \rceil$ and $\lfloor x + r \rfloor$, triangles of height u_n can be placed.[2] The cumulated area of all these triangles between $\lceil x + \alpha_{u_0} \rceil$ and $\lfloor x + r \rfloor$ is a lower bound on the area of the border of the first octant. Twice this cumulated area is given by

$$\left(\lfloor x + r \rfloor - \lceil x + \alpha_{u_n} \rceil\right) u_n + \sum_{i=0}^{n-1} \left(\lceil x + \alpha_{u_{i+1}} \rceil - \lceil x + \alpha_{u_i} \rceil\right) u_i.$$

After distributing the terms, one gets

$$\lfloor x + r \rfloor u_n - \lceil x + \alpha_{u_0} \rceil u_0 - \sum_{i=1}^{n} \lceil x + \alpha_{u_i} \rceil (u_i - u_{i-1}),$$

which can be minored by

$$(x + r - 1)u_n - (x + \alpha_{u_0} + 1)u_0 - \sum_{i=1}^{n} (x + \alpha_{u_i} + 1)(u_i - u_{i-1}).$$

Simplifying this lower bound removes the dependency on x. So the bound holds for all the other octants as well, which leads to the inequality

$$T/4 \geq (r - 2)u_n - \alpha_{u_0} u_0 - \sum_{i=1}^{n} \alpha_{u_i} (u_i - u_{i-1}).$$

[2] The last two abscissas may end up inverted: $\lfloor x + r \rfloor < \lceil x + \alpha_{u_n} \rceil$. Let us take the biggest i such that $\lceil x + \alpha_{u_i} \rceil = \lfloor x + r \rfloor$. The inversion causes us to count one too many triangle of slope u_i, while we are counting backward a single triangle of slope u_n. Since $u_n \geq u_i$, both miscounted triangles compensate themselves and do not invalidate the proof.

An interesting family of (u_i) sequences is $(i/j+1)_{0\le i\le (m-1)j}$ for any $j \ge 1$ and for any real number $m \ge 1$, as the inequality then becomes

$$T/4 \ge (r-2)m - \frac{r}{\sqrt{2}} - \frac{1}{j}\sum_{i=1}^{(m-1)j} \alpha_{i/j+1}.$$

The rightmost sum is a Riemann sum of the Riemann-integrable function α on the interval $[1, m]$, so it tends toward the integral when j tends to infinity. Since the inequality holds for any j, it also holds at the limit:

$$T/4 \ge (r-2)m - \frac{r}{\sqrt{2}} - \int_1^m \alpha_s \,\mathrm{d}s = (r-2)m - \frac{r}{\sqrt{2}} - \left(\sqrt{1+m^2} - \sqrt{2}\right) r.$$

The lower bound reaches its maximum for $m = \frac{r-2}{2\sqrt{r-1}}$. Injecting this special value of m in the formula gives the lower bound of Lemma 4. □

Corollary 1. *The radius of a disk containing k integer points is bigger than the positive root r of the quadratic equation*

$$\pi r^2 + 2r\left(2-\sqrt{2}\right) + \left(1 - k + 8\sqrt{\rho - 1}\right) = 0 \quad \textit{with } \rho = \sqrt{\frac{k-1}{\pi}}.$$

Proof. Let r be the minimal radius of a disk containing k integer points. Lemma 4 states the inequality

$$\pi r^2 + 2r\left(2-\sqrt{2}\right) > k - 1 - 8\sqrt{r-1}.$$

We can substitute for the rightmost r any of its upper bounds without invalidating the inequality above. In particular, we can use $\sqrt{(k-1)/\pi}$, in order to prove the corollary. □

For $k = 10^6$, this gives $r > 563.949$. This new bound is better than Chaix's bound for $k \le 759\,267\,778$, and better than the bound given by Lemma 2 for $k \le 1439$, which again shows that Lemma 2 is more useful for the computation of δ.

3. A tight analytic lower bound on r_k

Lemma 5. *For real $x \ge 0$ and arbitrary $\vec{c} = (c_1, c_2) \in \mathbb{R}^2$, let $C(x; \vec{c})$ denote the compact circular disc with center $\vec{c}$ and radius x, and $A(x; \vec{c})$ the number of integer points contained therein. Then it follows that, for $x \ge 5$,*

$$\left|A(x;\vec{c}) - \pi x^2\right| \le 7.213\, x^{2/3} + 1.5\, x^{1/2}\,.$$

Proof. We put $\varepsilon := \frac{b}{x^{1/3}}$, with a positive constant b at our disposal, and $K = (3\pi)^{-2/3}\varepsilon^{-1}$. Further, we write χ_M for the indicator function of any set $M \subseteq \mathbb{R}^2$, and $|\cdot|$ for the Euclidean norm in $\mathbb{R}^2$. The strategy is to approximate $\chi_{C(x;\vec{c})}$ by a smooth function, obtained by convolution (denoted by $*$) with $\delta := (\pi\varepsilon^2)^{-1}\chi_{C(\varepsilon;\vec{o})}$, where $\vec{o} = (0,0) \in \mathbb{R}^2$.

We first claim that

$$\chi_{C(x-\varepsilon;\vec{c})} * \delta \le \chi_{C(x;\vec{c})} \le \chi_{C(x+\varepsilon;\vec{c})} * \delta \tag{1}$$

throughout. A geometric intuition of these inequalities can be seen on Figure 3. Indeed, $(\chi_{C(y;\vec{c})} * \chi_{C(\varepsilon;\vec{o})})(\vec{u})$ is the area of the intersection between the two disks $C(y;\vec{c})$ and $C(\varepsilon;\vec{u})$. The constant $(\pi\varepsilon^2)^{-1}$ in the definition of δ ensures that the value $(\chi_{C(y;\vec{c})} * \delta)(\vec{u})$ is normalized between 0 and 1.

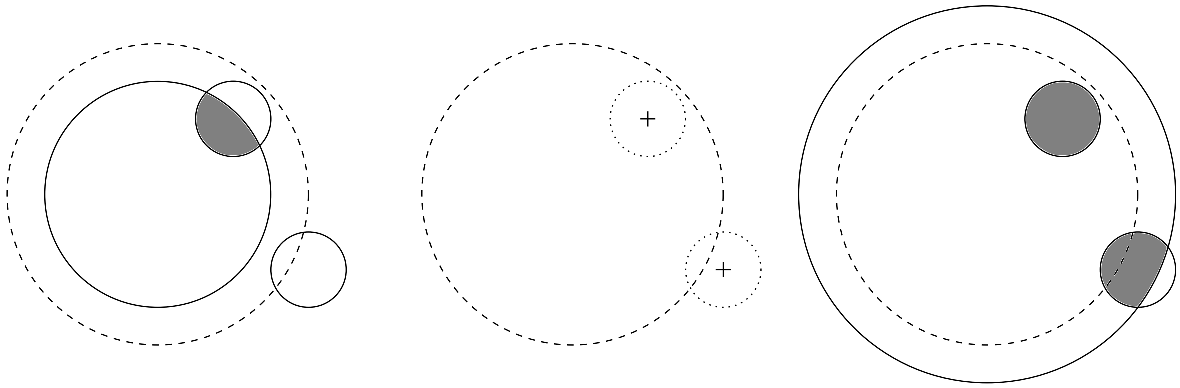

FIGURE 3. Intersections between $C(x \pm \varepsilon; \vec{c})$ and $C(\varepsilon; \vec{u})$. The grayed areas are proportional to the values of the lower and upper convolutions $\chi_{C(x\pm\varepsilon;\vec{c})} * \delta$ for the two points of the middle figure, one inside the disk, the other outside.

More formally, the two inequalities of Equation (1) can be verified by distinguishing two cases.

Case 1: $\vec{u} \notin C(x;\vec{c})$. Thus $|\vec{u}-\vec{c}| > x$. If $\delta(\vec{v}) \neq 0$, then $|\vec{v}| \leq \varepsilon$, hence $|\vec{u}-\vec{c}+\vec{v}| > x-\varepsilon$, therefore $\chi_{C(x-\varepsilon;\vec{c})}(\vec{u}+\vec{v}) = 0$. Thus $\delta(\vec{v})\chi_{C(x-\varepsilon;\vec{c})}(\vec{u}+\vec{v}) = 0$ for all $\vec{v} \in \mathbb{R}^2$, hence $(\chi_{C(x-\varepsilon;\vec{c})} * \delta)(\vec{u}) = 0$. The right-hand part of Equation (1) is trivial since $\chi_{C(x;\vec{c})}(\vec{u}) = 0$.

Case 2: $\vec{u} \in C(x;\vec{c})$. Thus $|\vec{u}-\vec{c}| \leq x$. If $\delta(\vec{v}) \neq 0$, then $|\vec{v}| \leq \varepsilon$, hence $|\vec{u}-\vec{c}+\vec{v}| \leq x+\varepsilon$, therefore $\chi_{C(x+\varepsilon;\vec{c})}(\vec{u}+\vec{v}) = 1$. Thus $\delta(\vec{v})\chi_{\mathbb{R}^2\setminus C(x+\varepsilon;\vec{c})}(\vec{u}+\vec{v}) = 0$ for all $\vec{v} \in \mathbb{R}^2$, hence $(\chi_{\mathbb{R}^2\setminus C(x+\varepsilon;\vec{c})} * \delta)(\vec{u}) = 0$, consequently $(\chi_{C(x+\varepsilon;\vec{c})} * \delta)(\vec{u}) = 1$. The left-hand part of Equation (1) is trivial since $\chi_{C(x;\vec{c})}(\vec{u}) = 1$.

We sum up Equation (1) over all integer points of $\mathbb{Z}^2$:

$$\sum_{\vec{m}\in\mathbb{Z}^2} (\chi_{C(x-\varepsilon;\vec{c})} * \delta)(\vec{m}) \leq A(x;\vec{c}) \leq \sum_{\vec{m}\in\mathbb{Z}^2} (\chi_{C(x+\varepsilon;\vec{c})} * \delta)(\vec{m}) \,.$$

By applying the multidimensional Poisson's formula (see Bochner [1]) to both sides, we get the following formula, where $\widehat{\cdot}$ denotes the Fourier transform:

$$\sum_{\vec{m}\in\mathbb{Z}^2} \widehat{\chi}_{C(x-\varepsilon;\vec{c})}(\vec{m})\widehat{\delta}(\vec{m}) \leq A(x;\vec{c}) \leq \sum_{\vec{m}\in\mathbb{Z}^2} \widehat{\chi}_{C(x+\varepsilon;\vec{c})}(\vec{m})\widehat{\delta}(\vec{m}) \,. \tag{2}$$

Obviously, $\widehat{\delta}(\vec{o}) = 1$, and $\widehat{\chi}_{C(x\pm\varepsilon;\vec{c})}(\vec{o}) = \pi(x\pm\varepsilon)^2$. Writing $\vec{z}\cdot\vec{u}$ for the standard inner product in $\mathbb{R}^2$, and $e(w) := e^{2\pi i w}$ as usual, we define, for $\vec{z} \in \mathbb{R}^2$,

$$I(\vec{z}) := \int\limits_{|\vec{u}|\leq 1} e(\vec{z}\cdot\vec{u})\mathrm{d}\vec{u} \,.$$

Then, for $\vec{o} \neq \vec{m} \in \mathbb{Z}^2$,

$$\widehat{\delta}(\vec{m}) = \frac{1}{\pi} I(\varepsilon\vec{m}) \,, \quad \widehat{\chi}_{C(x\pm\varepsilon;\vec{c})}(\vec{m}) = e(\vec{c}\cdot\vec{m})(x\pm\varepsilon)^2 I((x\pm\varepsilon)\vec{m}) \,.$$

Thus we conclude from Equation (2) that

$$\left|A(x;\vec{c}) - \pi x^2\right| \leq \pi(2x\varepsilon + \varepsilon^2) + \max_{R=x\pm\varepsilon} \Delta(R) \,, \tag{3}$$

where, for $R = x \pm \varepsilon$,

$$\Delta(R) := \frac{R^2}{\pi} \sum_{\vec{o} \neq \vec{m} \in \mathbb{Z}^2} |I(R\vec{m})| \, |I(\varepsilon\vec{m})| \, .$$

Evaluating $I(\vec{z})$, we get

$$|I(\vec{z})| = 2 \left| \int_{-1}^{1} \sqrt{1-v^2}\, e(|\vec{z}|v) \mathrm{d}v \right| = \frac{|J_1(2\pi|\vec{z}|)|}{|\vec{z}|} \, ,$$

where J_1 is a Bessel function of the first kind. Now

$$\max_{w>0} \left| J_1(w)\sqrt{w} \right| = 0.82503\ldots \, . \tag{4}$$

It is clear by inspection of a graph of $J_1(w)\sqrt{w}$ that the global maximum is attained at the first relative extremum $w_{\max} = 2.16587\ldots$; A rigorous proof can be based on the well-known asymptotics

$$J_1(w)\sqrt{w} = \sqrt{\frac{2}{\pi}} \cos\left(w - \frac{3\pi}{4}\right) + O(w^{-1}) \, ,$$

where the O-term can be bounded explicitly according to Gradshteyn and Ryzhik [3], formula 8.451. Note that $\sqrt{2/\pi} = 0.79788\ldots$.

Now Equation (4) implies that

$$|I(\vec{z})| \le 0.83(2\pi)^{-1/2}|\vec{z}|^{-3/2} < \frac{1}{3}|\vec{z}|^{-3/2} \, ,$$

hence, for $R = x \pm \varepsilon$,

$$|\Delta(R)| \le \frac{(x+\varepsilon)^{1/2}}{3\pi} \sum_{\vec{o} \neq \vec{m} \in \mathbb{Z}^2} |\vec{m}|^{-3/2} \min\left(\frac{1}{3}(\varepsilon|\vec{m}|)^{-3/2}, \pi\right) \, ,$$

taking into account also the trivial estimate $I(\varepsilon|\vec{m}|) \le \pi$. We split up this sum according to whether $|\vec{m}|$ is less or greater than $K = (3\pi)^{-2/3}\varepsilon^{-1}$, as defined earlier. Thus,

$$\begin{aligned} |\Delta(R)| &\le \frac{(x+\varepsilon)^{1/2}}{3\pi} \left(\pi \sum_{\vec{m} \in \mathbb{Z}^2:\ 1 \le |\vec{m}| \le K} |\vec{m}|^{-3/2} + \frac{1}{3\varepsilon^{3/2}} \sum_{\vec{m} \in \mathbb{Z}^2:\ |\vec{m}| > K} |\vec{m}|^{-3} \right) \\ &= (x+\varepsilon)^{1/2} \left(\frac{1}{3} \int_{1-}^{K+} \frac{\mathrm{d}A^*(w)}{w^{3/2}} + \frac{1}{9\pi\varepsilon^{3/2}} \int_{K+}^{\infty} \frac{\mathrm{d}A^*(w)}{w^3} \right) \, , \end{aligned}$$

where $A^*(w) := A(w;\vec{o}) - 1$, and Stieltjes integrals have been used. Integrating by parts, and using the inequality $(x+\varepsilon)^{1/2} < \sqrt{x} + \varepsilon/(2\sqrt{x})$, we infer that

$$|\Delta(R)| \le \left(\sqrt{x} + \frac{\varepsilon}{2\sqrt{x}}\right) \left(\frac{1}{2} \int_{1}^{K} \frac{A^*(w)}{w^{5/2}} \mathrm{d}w + \frac{1}{3\pi\varepsilon^{3/2}} \int_{K}^{\infty} \frac{A^*(w)}{w^4} \mathrm{d}w \right) . \tag{5}$$

It is easy to give a crude bound for $A^*(w)$: Observe that, for any $w \geq 0$,

$$\bigcup_{\vec{m}\in\mathbb{Z}^2:\ |\vec{m}|\leq w} \left(\vec{m} + \left[-\frac{1}{2}, \frac{1}{2}\right]^2\right) \subseteq C\left(w + \frac{\sqrt{2}}{2}; \vec{o}\right),$$

then it is immediate that

$$A^*(w) \leq \pi\left(w + \frac{\sqrt{2}}{2}\right)^2 - 1\,.$$

We use this in Equation (5), evaluate the integrals, recall Equation (3) and the definitions of K and ε. After carrying out all of these routine calculations, preferably supported by some symbolic computation software, we obtain a bound for $|A(x;\vec{c}) - \pi x^2|$ with leading term

$$\left(2\pi b + \frac{2(3\pi)^{2/3}}{3\sqrt{b}}\right) x^{2/3}\,.$$

Here the coefficient of $x^{2/3}$ attains its minimum for $b = \frac{1}{6}(\frac{17496}{\pi^2})^{1/9} = 0.382656\ldots$. With this choice of b, $K > 1$ for $x \geq 5$. We thus obtain

$$\left|A(x;\vec{c}) - \pi x^2\right| \leq 7.213\, x^{2/3} + 1.5\sqrt{x} - 2.9\, x^{1/3} + \frac{1.38\ldots}{x^{2/3}} + \frac{0.28\ldots}{x^{5/6}} - \frac{0.55\ldots}{x}\,.$$

From this, the assertion of the Lemma is immediate, since the sum of the last four terms is negative for $x \geq 5$. □

Remark. In its essence, this argument based on Fourier analysis and involving Poisson's formula is fairly standard; see, e.g., W. Müller [7] and the literature cited there. However, there are just a very few papers which pay attention to an explicit and very careful estimation of the constants involved: See, for instance, Krätzel and Nowak [6], where a weaker and less general version of Lemma 5 has been established.

4. Approximating radii by bisection

We describe here an alternate method, which is useful when k is too large for an exact computation of r_k, but still small enough such that one can outperform the analytic bound from Lemma 2. This method yields an enclosure $\ell \leq r_k \leq h$, where the bounds ℓ and h can be made arbitrarily tight given sufficient computer power, as it ultimately amounts to computing the optimal radius for each possible disk center.

For a given k, assume we want to show that $r_k > r$ for r fixed. If the center $x + iy$ of an optimal disk is known, this is easy: it suffices to count the number of integer points in the disk of center $x + iy$ and radius r. Now if we move slightly the center, the number of integer points will not change much. Moreover, if the center is in a small rectangle around $x + iy$, we can bound the number of integer points in the disk using interval arithmetic. Since it suffices to consider $0 \leq x \leq y \leq 1/2$ using symmetry, we can divide this domain in smaller subdomains, and hope that interval arithmetic will give a tight bound on the number of integer points. Consequently, assuming these computations show that all the disks of radius r have at most $k - 1$ integer points, we obtain $r_k > r$.

For example for $r = 563.873$, and with the whole square $0 \leq x, y \leq 1/2$, we get an upper bound of 999994 integer points, which gives the lower bound $r_k > r$ for $k \geq 999995$.

With 10 recursive subdivisions (5 for each coordinate, thus considering squares of width 2^{-6}) we get $564.169 < r_k < 564.190$ for $k = 10^6$.

In order to obtain an upper bound r on r_k, one just has to find one disk of radius r containing k or more integer points. More precisely, once an arbitrary point has been chosen as the disk center, a binary search on possible values of r will compute the minimal radius at this point — to get k or more integer points — and therefore an upper bound on r_k. In practice, corners of the subdivision used for getting a lower bound on r_k are chosen as disk centers.

The pseudo-code in Algorithm 1 sketches the algorithm used for finding a tight enclosure of r_k. Given k and an enclosure R of r_k, function `improve` returns another enclosure, hopefully tighter.

`nb_points`$(X = [\underline{x}, \overline{x}], Y = [\underline{y}, \overline{y}], r) =$

$$\sum_{j=\lceil \underline{x}-r \rceil}^{\lfloor \overline{x}+r \rfloor} \lfloor \overline{y} + h_j \rfloor - \lceil \underline{y} - h_j \rceil \qquad \text{with } h_j = \sup_{x \in [\underline{x}, \overline{x}]} \sqrt{r^2 - (x-j)^2}$$

`improve`$(k, R = [\underline{r}, \overline{r}]) =$
    assert $r_k \in R$
    let S a set of triples (X_i, Y_i, Z_i) initially empty
    let $\underline{z} = \overline{z} = \overline{r}$
    insert $([0, 0.5], [0, 0.5], R)$ into S
    while S is not empty
        extract an element (X_i, Y_i, Z_i) from S
        if $\overline{y_i} \leq \underline{x_i}$ or $\underline{z} \leq \underline{z_i}$ or `nb_points`$(X_i, Y_i, \underline{z}) < k$, then skip to next iteration
        let $\underline{r} = \underline{z_i}$ and $\overline{r} = \overline{z_i}$
        increase $\underline{r}$ while keeping `nb_points`$(X_i, Y_i, \underline{r}) < k$
        decrease $\overline{r}$ while keeping `nb_points`$([\underline{x_i}, \underline{x_i}], [\underline{y_i}, \underline{y_i}], \overline{r}) \geq k$
        if $X_i \times Y_i$ is small enough, then
            $\underline{z} \leftarrow \min(\underline{z}, \underline{r})$
            $\overline{z} \leftarrow \min(\overline{z}, \overline{r})$
        else
            split $X_i \times Y_i$ into two smaller rectangles $X' \times Y'$ and $X'' \times Y''$
            insert $(X', Y', [\underline{r}, \overline{r}])$ and $(X'', Y'', [\underline{r}, \overline{r}])$ into S
    return $[\underline{z}, \overline{z}]$

ALGORITHM 1. The bisection algorithm.

Here are a few remarks about this code. The `nb_points` function is specified to return an upper bound on the number of integer points contained in any disk of radius r and center contained in $X \times Y$. In the specific case where X and Y are singleton intervals (this case occurs when decreasing $\overline{r}$), the result is assumed to be exact in the algorithm.

The `improve` function stores in S all the rectangles that have yet to be handled. The variable $\overline{z}$ is an upper bound on r_k and it improves whenever a smaller disk containing k integer points (or more) is encountered. The variable $\underline{z}$ is a lower bound on the radius of all the disks containing at least k integer points whose center was in some already visited "small enough" rectangle. Both of them are initialized to a value sufficiently big (they could be set to $+\infty$) and they decrease over the course of the algorithm. The criteria we choose for stopping recursion is detailed in §5 along our numerical results.

All the triples (X_i, Y_i, Z_i) stored in the set S satisfy the following invariant: any minimal disk containing $\geq k$ integer points with a center in the rectangle $X_i \times Y_i$ has a radius contained in Z_i. For symmetry reasons, any triple with $\overline{y_i} < \underline{x_i}$ is redundant and thus skipped. In the algorithm, triples with $\overline{y_i} = \underline{x_i}$ are skipped too. Indeed, for the same symmetry reasons, the only interesting point from such a rectangle is $(\underline{x_i}, \overline{y_i})$; yet this point is also contained in several other rectangles, e.g., $[\underline{x_i} - \varepsilon, \underline{x_i}] \times [\underline{x_i} - \varepsilon, \underline{x_i}]$, that will not be skipped.

Triples are also skipped when $\underline{z} \leq \underline{z_i}$ or $\texttt{nb\_points}(X_i, Y_i, \underline{z}) < k$. These tests detect whether no disk can decrease the lower bound $\underline{z}$ further. Potentially, these triples might have still been able to improve the upper bound; skipping them is just a heuristic: the best improvement of the upper bound will happen when the lower bound is improved, since they are ultimately equal.

The performance of the algorithm will depend on the order triples are extracted from S and how $\underline{r}$ and $\overline{r}$ are refined. Our implementation (depth-first extraction, coarse-grained refinement) is probably not optimal.

5. Computation of δ

To obtain lower and upper bounds for δ, we proceed as follows. We choose an integer m_1 and we compute $s_{m_1} = \sum_{k=2}^{m_1} 1/(\pi r_k^2)$. Since r_k^2 is rational, πs_{m_1} is rational too and we compute it exactly by rational arithmetic. The only rounding error for s_{m_1} happens at the end of the computation, when we divide it by an approximation of π. We got the following timings on a 2.83Ghz Intel Core 2: r_{100000} was computed in 3.5s, r_{200000} in 12.1s, r_{500000} in 38.9s, and $r_{1000000}$ in 546.3s. As can be seen from these timings, the time complexity of computing exact values does not make it practical to go much further, so we stop at $m_1 = 10^6 - 1$. Using a variant of Theorem 1 at this point, we get the enclosure $1.8197 < \delta < 1.8206$, which is sufficient to disprove Gramain's conjecture but does not give much more information about the digits of δ than Gramain and Weber's result.

So we choose another integer $m_2 = 10^9 - 1$. For each k in $(m_1, m_2]$, we compute a lower bound for r_k using Lemma 4, and an upper bound using Lemma 3. We then refine these bounds with the bisection method described in Section 4. In our implementation, rectangles $X_i \times Y_i$ are bisected until their width reaches 2^{-17} or when the difference $\overline{r} - \underline{r}$ is small enough for the enclosure of $1/(\pi r_k^2)$ to be no wider than $10^{-5} k^{-1.1}$ — this bound was experimentally chosen to minimize the overall computation time. All the refined enclosures are computed and summed with double-precision interval arithmetic, 1000 at a time for parallelization purpose. Finally, all these partial sums are combined with enough precision to ensure that no additional rounding error occurs. So the overall rounding error due to summation is about $6 \cdot 10^{-13}$, hence negligible. In the end, this gives us an interval enclosing $s_{m_2} - s_{m_1}$, and thus s_{m_2}.

We use Theorem 1 to conclude:

$$1.81977613409613 < \delta < 1.81983226978634.$$

The width of this interval is about $56 \cdot 10^{-6}$. The contribution of the bisection algorithm is $50 \cdot 10^{-6}$, while the analytic estimate contributes the remaining $6 \cdot 10^{-6}$.

Acknowledgements. P. Zimmermann thanks Bruno Salvy who introduced him to the constant δ, and François Gramain for helpful discussions about his computation in [5] and for sending a copy of his personal notes. Experiments presented in this paper were carried out using the Grid'5000 experimental testbed, being developed under the INRIA ALADDIN development action with support from CNRS, RENATER and several Universities as well as other funding bodies (see `https://www.grid5000.fr/`). This work has been partly realized thanks to the support of the Région Lorraine and the CPER MISN TALC project. W. G. Nowak gratefully acknowledges support from the Austrian Science Fund (FWF) under project Nr. P20847-N18. Finally the authors thank the anynomous reviewer for his or her very useful comments.

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