THE SUM OF LAGRANGE NUMBERS

JONAH GASTER AND BRICE LOUSTAU

Abstract. Combining McShane's identity on a hyperbolic punctured torus with Schmutz's work on the Markov Uniqueness Conjecture (MUC), we find that MUC is equivalent to the identity

$$\sum_{n=1}^{\infty}(3-L_n) = 4-\varphi-\sqrt{2}$$

where L_n is the nth Lagrange number and $\varphi = \frac{1+\sqrt{5}}{2}$ is the golden ratio.

1. Preliminaries

1.1. **Lagrange and Markov numbers.** The *Lagrange numbers* $\mathcal{L} = \{L_n\}_{n=1}^{\infty} = \{\sqrt{5}, \sqrt{8}, \ldots\}$ are a sequence of real numbers that naturally arise in Diophantine approximation. Hurwitz's theorem states that for any irrational number x, there exists a sequence of rationals p_n/q_n converging to x with $\left|x - \frac{p_n}{q_n}\right| < \frac{1}{\sqrt{5}q_n^2}$. In this expression, $\sqrt{5}$ is optimal, as can be shown by taking $x = \varphi$ (the golden ratio). It turns out that when $x = \varphi$ and related numbers are excluded, $\sqrt{8}$ is the new best constant. By definition, $L_1 = \sqrt{5}$ is the first Lagrange number, $L_2 = \sqrt{8}$ is the second Lagrange number, etc.

The *Markov numbers* $\mathcal{M} = \{m_n\}_{n=1}^{\infty} = \{1, 2, 5, 13, \ldots\}$ are the positive integers that appear in a Markov triple, i.e. a solution $(x, y, z) \in \mathbb{Z}^3$ to the cubic

$$x^2 + y^2 + z^2 = 3xyz\,. \tag{1}$$

In 1880, Markov [Mar79, Mar80] discovered a remarkable connection between this cubic and the theory of binary quadratic forms, and proved the unexpected relation between Markov and Lagrange numbers:

$$L_n = \sqrt{9 - \frac{4}{m_n^2}}\,. \tag{2}$$

Using the Vieta involution $(x, y, z) \mapsto (x, y, 3xy - z)$, it is easy to see that for any Markov number m, one can always find a Markov triple $(x, y, z = m)$ with $0 < x \leqslant y \leqslant z$. The *Markov Uniqueness Conjecture* (MUC) asserts that such a triple is always unique. MUC was initially offered by Frobenius in 1913 [Fro13] and is notoriously difficult [Guy83]. For more context and detail, we refer to [Aig15, CF89].

1.2. **The sum of Lagrange numbers.** It is clear from (2) that L_n is an increasing sequence of positive numbers that converges to 3 when $n \to +\infty$. Moreover, we have $3 - L_n \sim \frac{2}{3m_n^2}$, and since $m_n \geqslant n$ (actually m_n is much greater, see § 3), the series $\sum_{n=1}^{\infty}(3 - L_n)$ is convergent. In this paper, we prove:

Theorem 1.1. *The Markov Uniqueness Conjecture holds if and only if*

$$\sum_{n=1}^{\infty}(3-L_n) = 4-\varphi-\sqrt{2}\,. \tag{3}$$

The proof is easily derived from the McShane identity on a hyperbolic punctured torus and a result of Schmutz regarding the well-known relationship between hyperbolic geometry and Markov numbers. It is nonetheless a striking identity, and could optimistically open a new path towards probing MUC.

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Remark 1.2. Several authors have explored similar ideas, for instance [Bow96], [LT07, §4.3].

Remark 1.3. Numerical computation confirms the identity (3) convincingly, as we shall see in § 3. This is not surprising since MUC has also directly been checked by computers for high values of n.

1.3. Markov numbers and the modular torus.

The beautiful relationship between Markov numbers and hyperbolic geometry was discovered by Gorshkov [Gor81] and Cohn [Coh55]. Let T^* denote the once-punctured torus, i.e. the topological surface obtained by removing a point from the torus T^2. For a certain hyperbolic metric on T^*, the lengths of simple closed geodesics on T^* are given by the Markov numbers. We briefly explain this connection and refer to e.g. [Ser85] for more discussion.

The *character variety* of the once-punctured torus is the cubic surface $\mathcal{X}$ defined by the equation

$$x^2 + y^2 + z^2 = xyz\,. \tag{4}$$

Hyperbolic metrics on T^* with finite volume correspond to real points of $\mathcal{X}$. Indeed, let $\pi_1(T^*) = \langle a, b\rangle$ where a and b are the standard generators of $\pi_1(T^2) \approx \mathbb{Z}^2$. Hyperbolic structures on T^* are parametrized by $x = \operatorname{tr}(A)$, $y = \operatorname{tr}(B)$, $z = \operatorname{tr}(AB)$ where $A, B \in \mathrm{SL}_2(\mathbb{R})$ are (lifts of) the holonomies of $a, b \in \pi_1(T^*)$. The condition that the metric has finite volume amounts to the peripheral curve $aba^{-1}b^{-1}$ having parabolic holonomy, i.e. $\operatorname{tr}(ABA^{-1}B^{-1}) = -2$. Using the classical trace relations in $\mathrm{SL}_2(\mathbb{R})$, this equation is rewritten $x^2+y^2+z^2 = xyz$. We refer to e.g. [Gol03] for more details on this correspondence.

The integer solutions $(x, y, z) \in \mathbb{Z}^3$ of (4) are clearly in bijection with Markov triples: x, y, z must all be divisible by 3, and the reduced triple $(x/3, y/3, z/3)$ verifies (1). Thus Markov triples are the integral points of $\mathcal{X}$ (up to 1/3). In fact, the mapping class group $\operatorname{Mod}(T^*)$ acts transitively on such triples, i.e. all corresponding hyperbolic tori are isometric. This hyperbolic torus is called the *modular torus* X, a 6-fold cover of the modular orbifold. Markov numbers can alternatively be described as one third of traces of simple closed geodesics on X:

$$3\,\mathcal{M} = \{3\,m_n,\, n \in \mathbb{N}\} = \{\tau(\gamma),\, \gamma \in \mathcal{S}\}$$

where we denote $\mathcal{S}$ the set of simple closed geodesics on X and $\tau(\gamma)$ the trace of the holonomy of $\gamma \in \mathcal{S}$.

It is natural to ask whether for any $m \in \mathcal{M}$, the geodesic γ such that $\tau(\gamma) = 3m$ is unique up to an isometry of X. It was proved by Schmutz [Sch96] that this statement is equivalent to MUC.

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2. Proof of the theorem

Greg McShane showed that, for any finite-volume hyperbolic metric on the punctured torus T^*,

$$\sum_{\gamma\in\mathcal{S}} \frac{1}{1+e^{\ell(\gamma)}} = \frac{1}{2}$$

where $\mathcal{S}$ is the set of simple closed geodesics and $\ell(\gamma)$ indicates the length of γ [McS98]. Recalling that the trace and length of γ are related by $\tau(\gamma) = 2\cosh(\ell(\gamma)/2)$, McShane's identity can be rewritten

$$\begin{aligned} 1 &= \sum_{\gamma} \frac{2}{1+e^{\ell(\gamma)}} = \sum_{\gamma} e^{-\ell(\gamma)/2}\operatorname{sech}(\ell(\gamma)/2) \\ &= \sum_{\gamma} \frac{2}{\tau(\gamma)+\sqrt{\tau(\gamma)^2-4}} \cdot \frac{2}{\tau(\gamma)} = \sum_{\gamma} 1 - \sqrt{1 - \frac{4}{\tau(\gamma)^2}}\,. \end{aligned} \tag{5}$$

When T^* with its hyperbolic metric is chosen to be the modular torus X, let us denote $m(\gamma) := \tau(\gamma)/3$ the associated Markov number (see § 1.3) and $L(\gamma) := \sqrt{9 - \frac{4}{m(\gamma)^2}}$ the associated Lagrange number. Reworking (5), McShane's identity on the modular torus is simply rewritten:

$$\sum_{\gamma\in\mathcal{S}} (3 - L(\gamma)) = 3\,. \tag{6}$$

It remains to investigate the fibers of the map $\gamma \mapsto L(\gamma)$ from simple closed geodesics on X to Lagrange numbers. It is not hard to show that all fibers are nonempty: this is because Vieta involutions act transitively on the Markov tree, and act as mapping classes on $\mathcal{S}$. By Schmutz's theorem [Sch96], MUC is equivalent to each fiber of $\gamma \mapsto L(\gamma)$ being the $\mathrm{Aut}(X)$-orbit of a single simple closed geodesic on X. To finish the proof of Theorem 1.1, we just need to count the number of elements of each orbit.

Lemma 2.1. *Let $\mathcal{S}_0 \subset \mathcal{S}$ indicate the six shortest geodesics on X, and let $\mathcal{S}_1 = \mathcal{S} - \mathcal{S}_0$. Each orbit $\mathrm{Aut}(X) \curvearrowright \mathcal{S}_0$ has three elements, and each orbit of $\mathrm{Aut}(X) \curvearrowright \mathcal{S}_1$ has six elements.*

Proof. There is an $\mathrm{Aut}(X)$-equivariant correspondence of $\mathcal{S}$ with lines in $H := H_1(X, \mathbb{Z})$. The standard generators a, b of $\pi_1(X) \approx \pi_1(T^*)$ (as in § 1.3) provide a basis of $H \approx \mathbb{Z}^2$. The image of the homomorphism $\mathrm{Aut}(X) \to \mathrm{PGL}(2, \mathbb{Z})$ is the dihedral group with six elements, generated by

$$r = \begin{pmatrix} 0 & 1 \\ -1 & -1 \end{pmatrix} \text{ and } \sigma = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

The actions of r and σ on $\mathbb{P}^1H$ have fixed points $\mathrm{Fix}(r) = \emptyset$ and $\mathrm{Fix}(\sigma) = \{[1:1], [1:-1]\}$. This implies that all simple closed geodesics on X have six images under the action of $\mathrm{Aut}(X)$, except for the two geodesics corresponding to ab and ab^{-1}, which have three such images apiece. These six geodesics are precisely the six shortest geodesics on X. □

Let us now prove Theorem 1.1, in fact the slightly more precise version:

Theorem 2.2. *We have $\sum_{n=1}^{\infty}(3 - L_n) \leqslant 4 - \varphi - \sqrt{2}$, with equality if and only if MUC holds.*

Proof. Recall that X denotes the modular torus and $\mathcal{S}$ the set of simple closed geodesics on X. Let $\mathcal{S}/\mathrm{Aut}(X)$ indicate the set of $\mathrm{Aut}(X)$-orbits in $\mathcal{S}$. By (6), the McShane identity on X is rewritten:

$$\sum_{\gamma\in\mathcal{S}} (3 - L(\gamma)) = \sum_{A\in\mathcal{S}/\mathrm{Aut}(X)} \sum_{\gamma\in A} 3 - L(\gamma) = 3\,.$$

By Lemma 2.1, the map $\gamma \mapsto L(\gamma)$ is 6-to-1 for $\gamma \in \mathcal{S}_1$ and 3-to-1 for $\gamma \in \mathcal{S}_0$. Therefore, we get

$$\left(6 \sum_{[\gamma]\in\mathcal{S}_1/\mathrm{Aut}(X)} + 3 \sum_{[\gamma]\in\mathcal{S}_0/\mathrm{Aut}(X)} \right) (3 - L(\gamma)) = 3\,.$$

The six curves in $\mathcal{S}_0$ are the shortest geodesics in $\mathcal{S}$, so the two Lagrange numbers they determine are the two smallest Lagrange numbers $L_1 = \sqrt{5}$ and $L_2 = \sqrt{8}$. The previous equality can be written

$$\left(6 \sum_{[\gamma]\in\mathcal{S}/\mathrm{Aut}(X)} (3 - L(\gamma)) \right) - 3\Big((3 - L_1) + (3 - L_2) \Big) = 3\,,$$

which we rewrite:

$$\sum_{[\gamma]\in\mathcal{S}/\mathrm{Aut}(X)} (3 - L(\gamma)) = 4 - \varphi - \sqrt{2}\,.$$

The map $[\gamma] \mapsto L(\gamma)$ from $\mathcal{S}/\mathrm{Aut}(X)$ to the set of Lagrange numbers $\mathcal{L} = \{L_n,\, n \in \mathbb{N}\}$ is onto, and one-to-one if and only if MUC holds (see discussion above Lemma 2.1). The conclusion follows. □

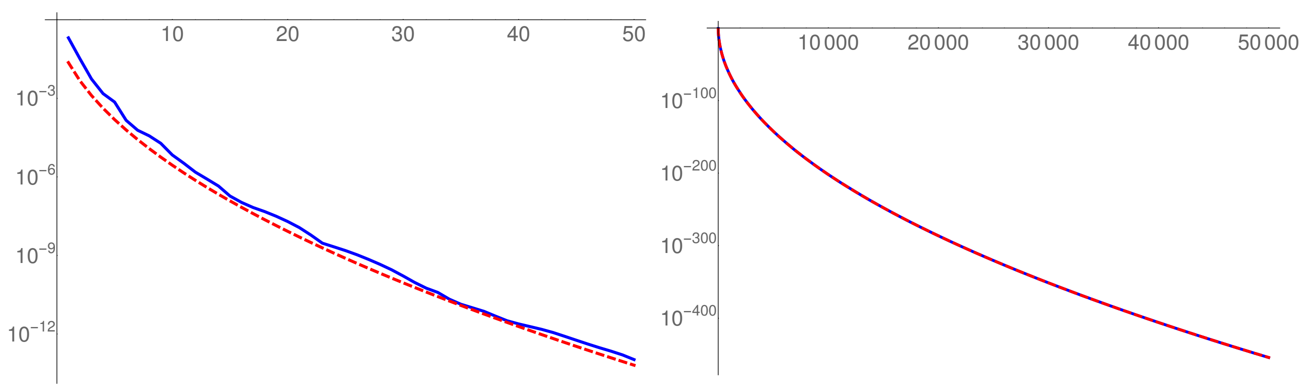
3. Numerical evidence

Numerical computation suggests that the series $\sum_{n=1}^{\infty}(3-L_n)$ indeed converges to $L = 4 - \varphi - \sqrt{2}$. Denoting $R_n := L - \sum_{k=1}^{n}(3-L_k)$ the presumed remainder, we find for instance $R_n \approx 7.34169 \times 10^{-455}$ for $n = 50\,000$.

Remark 3.1. Of course, one can also check MUC directly with an algorithm (see e.g. [Met15]). A short Python script took us less than a minute on a personal computer to check MUC for all Markov numbers m_n up to 10^{1000}, i.e. up to $n = 959\,047$. Nevertheless, it is nice to get a different confirmation.

Pushing the analysis further, we obtain new numerical evidence of Zagier's estimate $m_n \sim \frac{1}{3}e^{C\sqrt{n}}$ where $C = 2.3523414972\ldots$. Let us recall that this estimate is still open but was proved in weaker forms in [Zag82] and [MR95]. Elementary calculus involving the comparison of the remainder R_n with the integral $6\int_n^{+\infty} e^{-2C\sqrt{t}}\,\mathrm{d}t$ translates Zagier's estimate to $R_n \sim \frac{6\sqrt{n}}{C}e^{-2C\sqrt{n}}$. On Figure 1 it appears that the graph of R_n in Log scale is indeed asymptotic to the expected curve.

Remark 3.2 (Computer code). We wrote a simple recursive algorithm in Python to generate the list of Markov numbers. We then used Mathematica to compute the remainders R_n up to $n = 50\,000$ and plot the graphs. Our code is freely available on GitHub [js20].



(A) $n = 1 \ldots 50$.

(B) $n = 1 \ldots 50\,000$.

Figure 1. Numerical computation of the remainder $R_n = (4-\varphi-\sqrt{2}) - \sum_{k=1}^{n}(3-L_k)$. The dashed curve shows the expected asymptotic profile $\frac{6\sqrt{n}}{C}e^{-2C\sqrt{n}}$.

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Department of Mathematical Sciences, University of Wisconsin-Milwaukee
Email address: gaster@uwm.edu

Mathematisches Institut, Universität Heidelberg and Heidelberg Institute of Theoretical Studies
Email address: brice.loustau@uni-heidelberg.de