

THE SUM OF LAGRANGE NUMBERS

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

1. PRELIMINARIES

1.1. Lagrange and Markov numbers. The *Lagrange numbers* $\mathcal{L} = \{L_n\}_{n=1}^{\infty} = \{\sqrt{5}, \sqrt{8}, \dots\}$ 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 $x = \varphi$ (golden ratio). It turns out that when $x = \varphi$ is 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* $\mathcal{M} = \{m_n\}_{n=1}^{\infty} = \{1, 2, 5, 13, \dots\}$ are the positive integers that appear in a Markov triple, i.e. a solution $(x, y, z) \in \mathbb{Z}^3$ to the cubic

$$(1) \quad x^2 + y^2 + z^2 = 3xyz.$$

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:

$$(2) \quad L_n = \sqrt{9 - \frac{4}{m_n^2}}.$$

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, m) with $0 < x \leq y \leq m$. 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, 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 reals that converges to 3 when $n \rightarrow +\infty$. Moreover, known estimates on the growth rate of m_n (see § 3) imply that the series $\sum_{n=1}^{\infty} (3 - L_n)$ is convergent. In this paper, we show:

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

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

The proof of this theorem is easily derived from the McShane identity on a hyperbolic punctured torus using the well-known relationship between hyperbolic geometry and Markov numbers. It is nonetheless a striking identity, and could (very!) optimistically open a new path towards proving *MUC*.

Remark 1.2. Several authors have developed similar ideas, for instance [Bow96], [LT07, §4.3]. Such experts may well find the proof Theorem 1.1 evident.

Remark 1.3. Numerical computation confirms the value of this series quite convincingly, as we shall see in § 3. This is not surprising since *MUC* has also 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

$$(3) \quad x^2 + y^2 + z^2 = xyz.$$

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 $x = \text{tr}(A)$, $y = \text{tr}(B)$, $z = \text{tr}(AB)$ where $A, B \in \text{SL}_2(\mathbb{R})$ 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. $\text{tr}(ABA^{-1}B^{-1}) = -2$. Using the classical trace relations in $\text{SL}_2(\mathbb{R})$, 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 (3) are in bijection with Markov triples: x, y, z must all be divisible by 3, and $(x/3, y/3, z/3)$ verifies (1). Thus Markov triples are the integral points of the character variety (up to $1/3$). On the other hand, the mapping class group $\text{Mod}(T^*)$ 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. Since $\text{Mod}(T^*)$ acts transitively on simple closed curves, Markov numbers can alternatively be described as $1/3$ of traces of simple closed geodesics on X :

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

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

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

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. Reinvesting (4), McShane's identity on the modular torus is simply rewritten:

$$(5) \quad \sum_{\gamma \in \mathcal{S}} (3 - L(\gamma)) = 3.$$

It remains to investigate the fibers of the map $\gamma \mapsto L(\gamma)$ from simple closed geodesics on the modular torus X to Lagrange numbers. It is not hard to show that all fibers are nonempty unions of $\text{Aut}(X)$ -orbits. By Schmutz's theorem [Sch96], *MUC* is equivalent to the claim that each fiber of $\gamma \mapsto L(\gamma)$ is an $\text{Aut}(X)$ -orbit of a simple closed geodesic on X . To complete 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 $\text{Aut}(X) \curvearrowright \mathcal{S}_0$ has three elements, and each orbit of $\text{Aut}(X) \curvearrowright \mathcal{S}_1$ has six elements.*

Proof. There is an $\text{Aut}(X)$ -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 $\text{Aut}(X) \rightarrow \text{GL}(2, \mathbb{Z})$ 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 $\mathbb{P}^1 H$ have fixed points $\text{Fix}(r) = \emptyset$ and $\text{Fix}(\sigma) = \{[1 : 1], [1 : -1]\}$. This implies that all simple closed geodesics on X have six images under the action of $\text{Aut}(X)$, 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 . \square

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

Theorem 2.2. *We have $\sum_{n=1}^{\infty} (3 - L_n) \leq 4 - \varphi - \sqrt{2}$, 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 $\mathcal{O} = \mathcal{S}/\text{Aut}(X)$ indicate the set of $\text{Aut}(X)$ -orbits in \mathcal{S} . By (5), the McShane identity on X is rewritten:

$$\sum_{\gamma \in \mathcal{S}} (3 - L(\gamma)) = \sum_{A \in \mathcal{O}} \sum_{\gamma \in A} (3 - L(\gamma)) = 3.$$

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

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

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 rearranged:

$$\left(6 \sum_{[\gamma] \in \mathcal{O}} (3 - L(\gamma)) \right) - 3 \left((3 - L_1) + (3 - L_2) \right) = 3$$

which we rewrite:

$$\sum_{[\gamma] \in \mathcal{O}} (3 - L(\gamma)) = 4 - \varphi - \sqrt{2}.$$

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

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 $R_n \approx 4.242079 \times 10^{-287}$ for $n = 20\,000$. Figure 1 shows the graph of R_n in Log scale. Of course, *MUC* has also been checked directly for high values of n (at least for Markov numbers m_n up to 10^{140} , according to [Met15], i.e. $n \leq 18\,906$), but it is interesting to see 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 $C = 2.35234\dots$. 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 $6 \int_n^{+\infty} e^{-2C\sqrt{t}} dt$ 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 3.1. We wrote a simple recursive algorithm in Python to generate the list of Markov numbers. It takes a few seconds on a laptop to generate all Markov numbers up to 10^{400} , i.e. up to $n = 153\,665$. The graphs were computed and plotted in Mathematica. Our code is freely available on GitHub [js20].

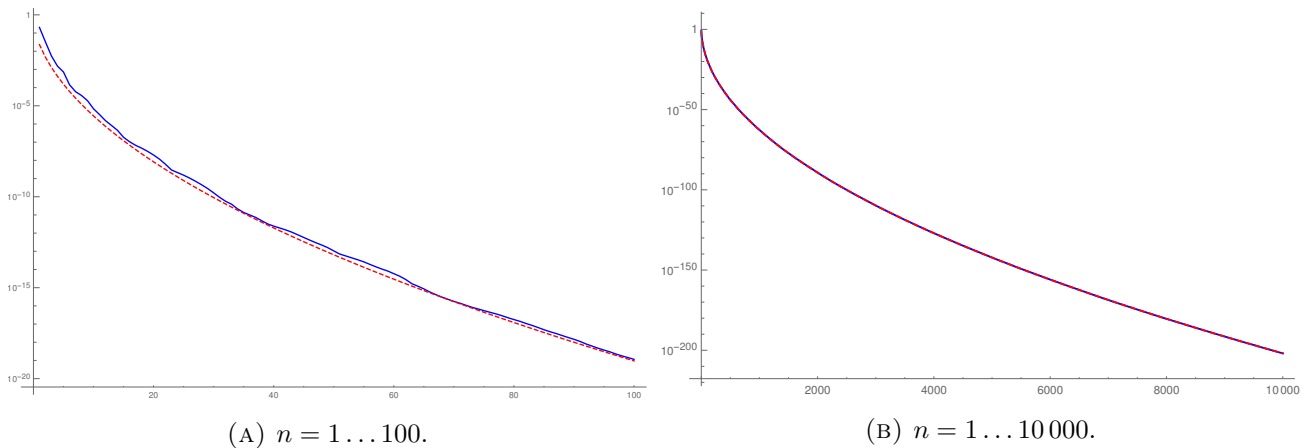


FIGURE 1. Numerical computation of the remainder $R_n = (4 - \varphi - \sqrt{2}) - \sum_{k=1}^n (3 - L_k)$. The dashed curve shows the expected asymptotic profile $\frac{6\sqrt{n}}{C}e^{-2C\sqrt{n}}$.

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