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 \( \mathcal{L} = \{L_n\}_{n=1}^{\infty} = \{\sqrt{5}, \sqrt{8}, \ldots\} \) 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 \( \frac{p_n}{q_n} \) 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

\[ x^2 + y^2 + z^2 = 3xyz \]

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:

\[ L_n = \sqrt{9 - \frac{4}{m_n^2}}. \]

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 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 \( m_n \geq n \) (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

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

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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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 $X$ defined by the equation

$$x^2 + y^2 + z^2 = xyz.$$  

Hyperbolic metrics on $T^*$ with finite volume correspond to real points of $X$. 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 (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 $X$ (up to 1/3). In fact, 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. Markov numbers can alternatively be described as one third 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 $\gamma$ 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 $\gamma$ [McS98]. Recalling that the trace and length of $\gamma$ are related by $\tau(\gamma) = 2 \cosh(\ell(\gamma)/2)$, McShane’s identity can be rewritten

$$1 = \sum_{\gamma} \frac{2}{1 + e^{\ell(\gamma)}} = \sum_{\gamma} e^{-\ell(\gamma)/2} \text{sech}(\ell(\gamma)/2)$$

$$= \sum_{\gamma} \frac{2}{\tau(\gamma) + \sqrt{\tau(\gamma)^2 - 4}} \cdot \frac{2}{\tau(\gamma)} = \sum_{\gamma} 1 - \sqrt{1 - \frac{4}{\tau(\gamma)^2}}.$$
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:

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

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 $\mathcal{L}$.

By Schmutz’ theorem [Sch96], MUC is equivalent to each fiber of $\gamma \mapsto L(\gamma)$ being the 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 $S_0 \subset S$ indicate the six shortest geodesics on $X$, and let $S_1 = S - S_0$. Each orbit Aut($X$) $\actson S_0$ has three elements, and each orbit of Aut($X$) $\actson S_1$ has six elements.

**Proof.** There is an Aut($X$)-equivariant correspondence of $S$ 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 Aut($X$) $\to$ PGL($2, \mathbb{Z}$) is the dihedral group with six elements, generated by

$$r = \begin{pmatrix} 0 & 1 \\ -1 & -1 \end{pmatrix} \quad \text{and} \quad \sigma = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \quad \text{The actions of $r$ and $\sigma$ on $\mathbb{P}^1H$ have fixed points $\text{Fix}(r) = \emptyset$ and $\text{Fix}(\sigma) = \{[1 : 1], [1 : -1]\}$. This implies that all simple closed geodesics on $X$ have six images under the action of Aut($X$), except for the two geodesics corresponding to $ab$ and $ab^{-1}$, which have three such images apiece. These six geodesics are precisely the six shortest geodesics on $X$.} \quad \Box$$

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 $S$ the set of simple closed geodesics on $X$. Let $S/\text{Aut}(X)$ indicate the set of Aut($X$)-orbits in $S$. By (6), the McShane identity on $X$ is rewritten:

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

By Lemma 2.1, the map $\gamma \mapsto \tau(\gamma)$ is 6-to-1 for $\gamma \in S_1$ and 3-to-1 for $\gamma \in S_0$. Therefore, we get

$$\left(6 \sum_{[\gamma] \in S_1/\text{Aut}(X)} + 3 \sum_{[\gamma] \in S_0/\text{Aut}(X)} \right) (3 - L(\gamma)) = 3.$$

The six curves in $S_0$ are the shortest geodesics in $S$, 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

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

which we rewrite:

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

The map $[\gamma] \mapsto L(\gamma)$ from $S/\text{Aut}(X)$ 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. \quad \Box
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 $n = 50000$.

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 $n = 959047$. 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 $\int_{n}^{+\infty} e^{-2C\sqrt{t}} \, dt$ 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 3.2 (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 $n = 50000$ and plot the graphs. Our code is freely available on GitHub [js20].

![Figure 1](https://github.com/seub/LagrangeSeries)

**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 $\frac{6\sqrt{n}}{e^{C\sqrt{n}}}$.

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