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 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 $x = \mathrm{tr}(A)$, $y = \mathrm{tr}(B)$, $z = \mathrm{tr}(AB)$ 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. $\mathrm{tr}(ABA^{-1}B^{-1}) = -2$. 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 $\mathrm{Mod}(T^*)$ 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

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

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 $\mathbb{P}^1 H$ 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. □

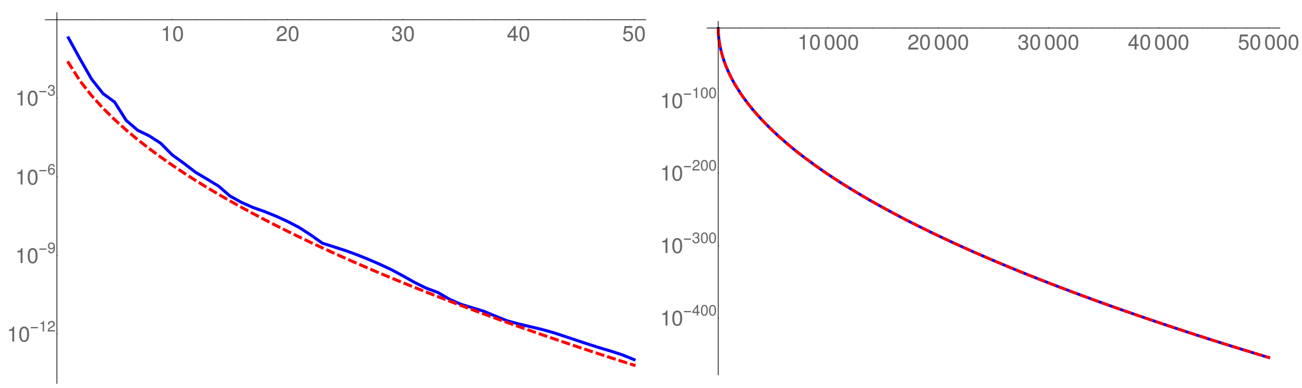
3. Numerical evidence

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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