APPROXIMATIONS OF THE LAGRANGE AND MARKOV SPECTRA

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Abstract. We describe a polynomial time algorithm providing finite sets arbitrarily close (in Hausdorff topology) to the Lagrange and Markov spectra.

1. Introduction

Given a positive real number \( \alpha \) we define the best constant of Diophantine approximation of \( \alpha \) as

\[
L(\alpha) := \limsup_{p,q \to \infty} \frac{1}{|q(\alpha - p)|}
\]

where \( p \) and \( q \) are bound to be positive integers. The Lagrange spectrum \( L \) is the set \( \{L(\alpha) : \alpha \in \mathbb{R} \setminus \mathbb{Q}\} \).

Perron [Per21] showed that if \( \alpha = [a_0; a_1, \ldots] \) is the continued fraction expansion of \( \alpha \) then

\[
L(\alpha) = \limsup_{n \to \infty} (a_n + [0; a_{n-1}, a_{n-2}, \ldots, a_0] + [0; a_{n+1}, a_{n+2}, \ldots]).
\]

In other words, one can equivalently define the Lagrange spectrum on the bi-infinite shift \( \Sigma = \{1, 2, 3, \ldots\}^\mathbb{Z} \).

More concretely, let us define the height function \( \lambda_0 : \Sigma \to \mathbb{R}_+ \) by

\[
\lambda_0(\underline{a}) = a_0 + [0; a_{-1}, a_{-2}, \ldots] + [0; a_1, a_2, \ldots]
\]

where \( \underline{a} = (a_n)_{n \in \mathbb{Z}} \). We have

\[
L = \left\{ \limsup_{n \to +\infty} \lambda_0(\sigma^n(\underline{a})) : \underline{a} \in \Sigma \right\},
\]

where \( \sigma : \Sigma \to \Sigma \) is the shift map. The Markov spectrum can be defined similarly as

\[
M = \{M(\underline{a}) : \underline{a} \in \Sigma \}
\]

where \( M(\underline{a}) = \sup_{n \in \mathbb{Z}} \lambda_0(\sigma^n(\underline{a})) \).

\( L \) and \( M \) are subsets of \( \mathbb{R}_+ \) which were first systematically studied by Markov [Ma1], [Ma2] circa 1879. It is known that the Lagrange, resp. Markov spectrum is the closure of the values of \( M(\underline{a}) \) for periodic, resp. ultimately periodic sequences \( \underline{a} \) (see [CF89, Chapter 3]): in particular, \( L \) and \( M \) are closed sets with \( L \subset M \). Nevertheless, they do not coincide [Fre68]. Actually, the second and third authors of the present text proved recently [MaMo1] that the Hausdorff dimension \( HD(M \setminus L) \) of \( M \setminus L \) satisfies

\[
0.53128 < HD(M \setminus L) < 0.986927.
\]

Also, it was shown by Freiman [Fre73] and Schecker [Sch77] that \( L \) contains the half-line \([\sqrt{21}, +\infty)\).

We recommend consulting Cusick–Flahive book [CF89] for a detailed account of several features of these fascinating spectra describing also the cusp excursions of geodesics on the modular surface.

Our aim in this article is to approximate \( L \) and \( M \) by mean of computations. More precisely we will be doing so by constructing finite sets that are close in Hausdorff distance. Let \( X \) and \( Y \) be set of real numbers. We say that \( X \) and \( Y \) are \( \varepsilon \)-close (in Hausdorff distance) if

\[
\forall x \in X, \exists y \in Y, |x - y| < \varepsilon \quad \text{and} \quad \forall y \in Y, \exists x \in X, |x - y| < \varepsilon.
\]

Theorem 1. Let \( R > 0 \). Then there exists an algorithm that given \( Q \) provide finite sets \((1/Q)\)-close respectively to the Lagrange and Markov spectrum in \([0, R]\). There exists a constant \( 0 < d_R < 1 \) such that its running time is \( O(Q^{3d_R}) \) with the following upper bounds

- \( d_R < 0.532 \) for \( R \leq \sqrt{13} \approx 3.606 \),
- \( d_R < 0.706 \) for \( R \leq 2\sqrt{5} \approx 4.772 \),
- \( d_R < 0.789 \) for \( R \leq \sqrt{21} \approx 4.583 \).

The numbers \( d_R \) above are actually Hausdorff dimensions of the sets \( E_K, \ 2 \leq K \leq 4 \), of real numbers whose continued fraction expansions only contain the digits from 1 to \( K \).

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Remark 2. As we mentioned already, $L$ contains the half line $[\sqrt{21},+\infty)$ and it does not make any sense to consider values of $R$ larger than $\sqrt{21}$.

Among our several motivations to get Theorem 1 we would like to mention that an efficient algorithm producing high resolution drawings of $L$ and $M$ could potentially lead the way to solve some longstanding questions such as Bernstein conjecture [Be73] that $[4,1,4,52] \subset L$. As it turns out, the algorithm provided by Theorem 1 is not sufficiently powerful yet to put us in good position to attack any of these questions. We hope to pursue this discussion in future works.

Let us now describe the main ideas of the algorithm in Theorem 1. Because we consider Lagrange and Markov values in the interval $[0, R]$ we can restrict to continued fractions with partial quotients $\{1,2,\ldots,\lfloor R \rfloor\}$. Let $\Sigma_K := \{1,\ldots, K\}^\mathbb{Z}$. We denote by $L_K$ and $M_K$ respectively the Lagrange and Markov spectra restricted to the shift $\Sigma_K$, that is $L_K = \{L(\vec{a}) : \vec{a} \in \Sigma_K\}$ and $M_K = \{M(\vec{a}) : \vec{a} \in \Sigma_K\}$. For each $K$, the relation $L_K \subset M_K$ holds.

The first step of the algorithm consists in constructing a subshift of finite type $\Sigma_{K,Q}$ on the alphabet $\{1,\ldots, K\}$ depending on the quality of approximation $Q$. $\Sigma_{K,Q}$ is the set of infinite paths on a graph $G_{K,Q}$ and each edge of $G_{K,Q}$ corresponds to a certain cylinder set $\vec{b} = (b_{-m},\ldots, b_0,\ldots, b_n)$ of the shift $\Sigma_{K,Q}$ satisfying

$$\sup_{\vec{a} \in \vec{b}} \lambda_0(a) - \inf_{\vec{a} \in \vec{b}} \lambda_0(a) < \frac{1}{Q}. \tag{1}$$

In the above equation and all along the text we identify a finite pointed word $\vec{b}$ (ie with a distinguished origin $b_0$) and there associated cylinder set $\{\vec{a} \in \Sigma_K : \forall k \in \{-m,\ldots, n\}, a_k = b_k\}$.

We turn the graph $G_{K,Q}$ into a weighted graph by considering on the edge associated to $\vec{b}$ the weight $\frac{2}{\inf_{\vec{a} \in \vec{b}} \lambda_0(\vec{a}) + \sup_{\vec{a} \in \vec{b}} \lambda_0(\vec{a})}$. The weighted graph $G_{K,Q}$ provide an approximation of the shift $\Sigma_K$ together with the height function $\lambda_0$. The condition (1) gives upper bound on the quality of approximation.

The rest of the algorithm consists in studying directly on the graph $G_{K,Q}$ the discrete analogue of Lagrange and Markov spectrum. The overall complexity of the algorithm is governed by the size of $G_{K,Q}$. It is not so surprising that this is related to the Hausdorff dimension of the Lagrange and Markov spectra.

The algorithm developed in this article has been implemented by the first author using the computer algebra software SageMath [S+09]. Part of the code has also been optimized using the Python-to-C compiler Cython [Cyt] and the figures were generated with Matplotlib (see [Hu07]). The code is publicly available at https://plmlab.math.cnrs.fr/delecroix/lagrange.

Let us describe the organization of the article. In Section 2 we compute some auxiliary intervals containing the sets $L_K$ for $1 \leq K \leq 4$. In Section 3 we describe the weighted directed graphs $G_{K,Q}$ and their basic properties. After that, in Section 4 we provide the discrete analogue of Lagrange and Markov spectra on a weighted directed graph. In Section 5 we justify that the discrete spectrum provide $(1/Q)$-approximation of the original Lagrange and Markov spectra. The main ingredient for the running time complexity is contained in Theorem 13 from Section 6. Finally, for the sake of comparison with Theorem 1 we consider in Section 7 the alternative idea of approaching the Lagrange spectrum via periodic orbits in $\{1,\ldots, K\}^\mathbb{Z}$. Unfortunately our complexity bounds for the resulting algorithm are very poor: roughly speaking, we are currently obliged to perform calculations with $4^{Q^n}$ periodic orbits in order to rigorously ensure that we got a $(1/Q)$-dense subset of $L$!

The final Section 8 contains some rigorous pictures obtained via the algorithm from Theorem 1.

2. Preliminary bounds on $L_K$

In this entire article, $K$ is an integer $1 \leq K \leq 4$ except when it is explicitly stated otherwise. Recall that $L_K$ is the set of Lagrange values $L(\vec{a})$ when $\vec{a}$ is restricted to the shift $\Sigma_K = \{1,\ldots, K\}^\mathbb{Z}$. It is easy to see that the smallest and largest values of $L_K \setminus L_{K-1}$ are respectively $L(\vec{K})$ and $L(\vec{1},\vec{K})$ where for a finite word $\vec{u}$ we denote $\overrightarrow{u}$ the associated periodic biinfinite word.

4In fact, despite the fact that some heuristic arguments from the projection theory of fractal sets are compatible with the presence of intervals in $L$ before the so-called Hall’s ray, Berstein conjecture is somewhat surprising to us because it propose a concrete relatively large interval before Hall’s ray.
The points
\[
\begin{align*}
[0; 1] &= \frac{\sqrt{3} - 1}{2} & \simeq 0.6180 \\
[0; 2] &= \frac{\sqrt{2} - 1}{2} & \simeq 0.4142 \\
[0; 3] &= \frac{\sqrt{13} - 3}{2} & \simeq 0.3028 \\
[0; 4] &= \frac{\sqrt{5} - 2}{2} & \simeq 0.2361
\end{align*}
\]
and
\[
\begin{align*}
[0; 2; 1] &= \frac{\sqrt{3} - 1}{2} & \simeq 0.3660 \\
[0; 3; 1] &= \frac{\sqrt{21} - 3}{6} & \simeq 0.2638 \\
[0; 4; 1] &= \frac{\sqrt{1} - 1}{2} & \simeq 0.2071 \\
[0; 1; 3] &= \frac{\sqrt{21} - 3}{2} & \simeq 0.7913 \\
[0; 1; 4] &= 2\sqrt{2} - 2 & \simeq 0.8284
\end{align*}
\]
allow to determine the intervals containing \( L_K \setminus L_{K-1} \) for \( 1 \leq K \leq 4 \), see Figure 1.

The ranges of \( R \) for which we provide upper bounds on \( d_R \) in Theorem 1 are visible on Figure 1.

- \( L(2, 1) = \sqrt{13} \) is the maximum of \( L_3 \).
- \( L(4, 1) = 2\sqrt{2} \) is the maximum of \( L_4 \setminus L_3 \).

Let us also mention that \( L(3, 1) = 2\sqrt{11} \) is the maximum of \( L_4 \).

3. Shifts of finite type

In this section we construct the graphs \( G_{K,Q} \) and their associated shifts of finite type \( \Sigma_{K,Q} \). The construction requires intermediate graphs \( \Sigma_{K,Q}^{\pm} \) that are associated to the one-sided shift \( \Sigma_{K}^+: \{1, \ldots, K\}^N \).

3.1. \((1/Q)-cylinders for the Gauss map.\) In this section we consider approximations of \( \Sigma_{K}^+ \) by shift of finite type. The continued fraction embeds the shift \( \Sigma_{K}^+ \) into \( \mathbb{R} \) as
\[
\Sigma_{K}^+: \mathcal{A} = (a_n)_{n \geq 1} \rightarrow \mathbb{R}_+ \quad \leftrightarrow \quad [0; a_1, a_2, \ldots]
\]
The image of \( \Sigma_{K}^+ \) under this map is a Cantor set \( E_K \).

For a finite (one sided) cylinder \( \tilde{b} = (b_1, \ldots, b_n) \) for the Gauss map we use the notation
\[
\frac{p_k(\tilde{b})}{q_k(\tilde{b})} = \frac{1}{b_1 + \frac{1}{b_2 + \ldots + \frac{1}{b_k}}}.
\]
A cylinder \( \tilde{b} \in \{1, \ldots, K\}^n \) projects on \([0, 1]\) on a subset \( I_K(\tilde{b}) \cap E_K \) where \( I_K(\tilde{b}) \) is the interval with extremities
\[
\frac{p_n(\tilde{b}) + \alpha_{K}^-}{q_n(\tilde{b}) + \alpha_{K}^+} \quad \text{and} \quad \frac{p_n(\tilde{b}) + \alpha_{K}^-}{q_n(\tilde{b}) + \alpha_{K}^+}
\]
where \( \alpha_{K}^- = [0; K, 1] \) and \( \alpha_{K}^+ = [0; 1, K] \). The values of \( \alpha_{K}^- \) and \( \alpha_{K}^+ \) for \( K \in \{1, 2, 3, 4\} \) were computed in Section 2.

Note that depending on the parity of the length \( |\tilde{b}| \) of \( \tilde{b} \) one or the other is the left handside.
of the interval. The diameter of \( I_K(\vec{b}) \) is

\[
\text{diam}_K(\vec{b}) := \frac{(\alpha_K^+ - \alpha_K^-)}{(q_{\alpha}(\vec{b}) + \alpha_K^+ q_{\alpha-1}(\vec{b}))(q_{\alpha}(\vec{b}) + \alpha_K^- q_{\alpha-1}(\vec{b}))}.
\]

Note that it is slightly smaller than the size \( \text{diam}(\vec{b}) = \frac{1}{q_{\alpha}(q_{\alpha} + q_{\alpha-1})} \) when we do not restrict to the subshift \( \{1, \ldots, K\}^\mathbb{N} \). Now given \( Q \) we consider the following set of cylinders

\[
C_{K,Q} := \left\{ \vec{b} \in \{1, \ldots, K\}^+: \text{diam}_K(\vec{b}) \leq \frac{1}{Q} \right\}
\]

where \( \vec{b} \) denotes the prefix of length \(|\vec{b}| - 1\) of \( b \) and \( \text{diam}_K(\vec{b}) \) is defined in (2).

First, notice that if \( \vec{b} \in C_{K,Q} \) then no proper prefix of \( \vec{b} \) belongs to \( C_{K,Q} \) and that any proper suffix of \( \vec{b} \) is a prefix of some element in \( C_{K,Q} \). The set \( C_{K,Q} \) can naturally be thought as the leaves of a tree rooted at the empty word \( \varepsilon \) and where the edges correspond to adding a letter to the right. Namely, consider the set \( \overline{C}_{K,Q} \) to be the union of \( C_{K,Q} \) and all prefixes of elements of \( C_{K,Q} \). The tree has vertex \( \overline{C}_{K,Q} \) and we put an oriented edge from \( u \) to \( v \) if \( u \) is the prefix of length \(|v| - 1\) of \( v \).

We add edges on this tree corresponding to the so called suffix links. For each \( w \in C_{K,Q} \) we add an edge from \( w \) to its suffix of length \(|w| - 1 \). As we already mentioned, this suffix belongs necessarily to \( \overline{C}_{K,Q} \). One can visualize the tree and the suffix links of \( C_{2,20} \) on Figure 2.

![Figure 2. The tree of \( T_{2,20} \) and the suffix links (in red) on the left. The graph \( G^+_{2,20} \) on the right with the prolongation edges in black and the shift edges in red.](image)

Now we define the set \( V^+_{K,Q} \) as the set of endpoints of the suffix links (in other words the maximal non-trivial suffixes of elements of \( C_{K,Q} \)). We consider two kinds of edges on the vertex set \( V^+_{K,Q} \). First, for each (oriented) path in the tree \( T_{K,Q} \) between pairs of vertices \( V^+_{K,Q} \) we add an edge in \( G^+_{K,Q} \). We call such edge a prolongation edge (they are in black on Figure 2). Secondly, for each suffix link \( s \) from \( u \) to \( v \) in \( T_{K,Q} \), there is a unique vertex \( w \) in \( V^+_{K,Q} \) and a path from \( w \) to \( v \) that avoids any other element from \( V^+_{K,Q} \). We add an edge from \( w \) to \( v \) that we call a shift edge.

Each edge carries a label that is a finite word on \( \{1, \ldots, K\} \) (possibly empty). They are directly induced from the tree \( T_{K,Q} \) for which each edge carry a letter. Each prolongation edge in \( G^+_{K,Q} \) already carries a letter and we keep this letter as a label. Each shift edge is made of the concatenation of a path \( w \to u \) and a suffix link and we associate to this edge the label of the path \( w \to u \) in the tree \( T_{K,Q} \).

**Lemma 3.** For any \( K \) and \( Q \) the graph \( G^+_{K,Q} \) recognize the shift \( \{1, \ldots, K\}^\mathbb{Z} \): for any biinfinite word \( w \in \Sigma_K \) there exists a unique biinfinite path \( \gamma \) in \( G^+_{K,Q} \) so that \( w \) can be read along \( \gamma \).
Remark 4. The construction of the graphs $G^+_{K,Q}$ from $C_{K,Q}$ can be generalized to any set of words with the same properties (every word in $\Sigma^+_{K}$ has a prefix in the set and no proper prefix of an element of the set is contained in the set). If we had used instead of $C_{K,Q}$ the set of words of given combinatorial length we would have obtain the de Bruijn graph $[11B3]$. 

3.2. From $G^+_{K,Q}$ to $G_{K,Q}$. Now that we have the graph $G^+_{K,Q} = (V^+_{K,Q}, E^+_{K,Q})$ at hand we explain the construction of $G_{K,Q}$. Similarly to $G^+_{K,Q}$, the graph $G_{K,Q}$ has two kinds of edges: prolongation edges and shift edges. The shift edges are in bijection with $C_{K,Q} \times \{1, \ldots, K\} \times C_{K,Q}$. Let $(p, a_0, s) \in C_{K,Q} \times \{1, \ldots, K\} \times C_{K,Q}$. Let $u$ and $v$ be the source and target of the shift edge associated to $s$ in $G^+_{K,Q}$. By construction, if $s = (s_1, \ldots, s_n)$ then $u = (s_1, \ldots, s_k)$ and $v = (s_2, \ldots, s_n)$ for some $0 \leq k \leq n$. The source of the edge corresponding to $(p, a_0, s)$ in $G_{K,Q}$ is $(p, a_0, s)$ and its target is $(p', s_1, v)$ where $p'$ is the unique element in $C_{K,Q}$ that is a prefix of $ap$.

We now describe prolongation edges. To each prolongation edge in $G^+_{K,Q}$ from $u = (s_1, \ldots, s_k)$ to $v = (s_1, \ldots, s_{k+1})$ we associate for each $p$ in $C_{K,Q}$ and each $a_0$ in $\{1, \ldots, K\}$ a prolongation edge from $(p, a_0, u)$ to $(p, a_0, v)$.

For the shift edge corresponding to $(p, a_0, s)$ we associate the weight

$$F((p, a_0, s)) = a_0 + \text{mid}_K(p) + \text{mid}_K(s)$$

where $\text{mid}_K(\vec{b})$ is the middle of the interval determined by a cylinder $\vec{b} = (b_1, \ldots, b_n)$ given by

$$\text{mid}_K(\vec{b}) = \frac{1}{2} \left( \frac{p_n(\vec{b}) + \alpha^+_K p_{n-1}(\vec{b})}{q_n(\vec{b}) + \alpha^+_K q_{n-1}(\vec{b})} + \frac{p_n(\vec{b}) + \alpha^-_K p_{n-1}(\vec{b})}{q_n(\vec{b}) + \alpha^-_K q_{n-1}(\vec{b})} \right).$$

We give weight 0 to each prolongation edge.

As before, the biinfinite paths on edges of $G_{K,Q}$ define a subshift of finite type.

Lemma 5. For each $Q$, the graph $G_{K,Q}$ recognizes the subshift $\Sigma_K$. Moreover, for any shift edge in $G_{K,Q}$ associated to the cylinder $(p, a_0, s) \in C_{K,Q} \times \{1, \ldots, K\} \times C_{K,Q}$ we have

$$\sup_{\vec{a} \in (p, a_0, s)} |\lambda_0(\vec{a}) - F((p, a, s))| \leq \frac{1}{Q}.$$  

Proof. Recall that the weights defined in (4) are in between the extremal possible values of $\lambda_0(\vec{a})$ in the cylinder $(p, a_0, s)$. But $p$ and $s$ are in $C_{K,Q}$ constructed in Section 3.2 and were chosen so that the corresponding image under the continued fraction map have diameter $< 1/Q$. Hence for each of $\text{mid}_K(p)$ and $\text{mid}_K(s)$ we are off by at most $1/(2Q)$ so that $a_0 + \text{mid}_K(p) + \text{mid}_K(s)$ is off by at most $1/Q$. □

Remark 6. Since the Gauss map $g(x) = \{1/x\}$ has derivative $g'(x) = -1/x^2$, we have $(\alpha^+_K)^{2n} \leq \frac{\text{diam}_K(\vec{b})}{(\alpha^-_K - \alpha^+_K)} \leq (\alpha^-_K)^{2n}$ for any $b \in \{1, \ldots, K\}^n$.

In particular, an alternative way of constructing a subshift would have been to pick all possible cylinder of combinatorial length $n$ (where $n$ is chosen large enough so that all diameters are smaller than $(1/Q)$), but this would have lead to a larger set of cylinders.

4. Lagrange and Markov edges in weighted directed graphs

Let $G$ be a weighted directed graph. We denote $V(G)$ and $E(G)$ respectively the vertices and edges of $G$ and $w : E(G) \to \mathbb{R}$ the weight function. The codomain of the weight function needs not be $\mathbb{R}$, any totally ordered set would do.

We call an edge $e$ in $G$ to be a Lagrange edge if there exists a cycle $\gamma$ in $G$ that passes through $e$ and so that the weight of the edge $e$ is maximal among the weights of edges in $\gamma$. An edge is called a Markov edge if there exist two cycles $\gamma^-$ and $\gamma^+$ and a path $p$ from $\gamma^-$ to $\gamma^+$ so that the edge $e$ is maximal among the weights of edges in $\gamma^- \cup p \cup \gamma^+$. The definition is illustrated with a simple example on Figure 3.

Figure 3. A weighted graph with its Lagrange edges in red and its single Markov but not Lagrange edge in blue.

A simple approach for computing these edges is to test for each edge whether it is Lagrange or Markov.
Theorem 7. Given $G$ a directed graph and $w : E(G) \to \mathbb{R}$ and an edge $e$ of $G$. Determining whether $e$ is Lagrange or Markov has complexity $O(m)$ where $m$ is the number of edges in $G$.

Proof. Let $e$ be an edge and $u$ and $v$ its source and target. Then $e$ is a Lagrange edge if and only if there is a path from $v$ to $u$ with maximum edge weight $w(e)$. To compute that, one can simply do a depth-first search on edges with weight not greater than $w(e)$. Hence testing whether a single edge is Lagrange is $O(m)$. Now $e$ is a Markov edge if one can build a path connected to a cycle (both backward and forward). Similarly, one can detect such cycle with two depth first searches. In both cases, the search is bounded by the number of edges in the graph $G$. □

As a consequence of Theorem 7 the complexity of computing all Lagrange and Markov edges in a given graph $G$ has complexity $O(m^2)$ where $m$ is the number of edges in $G$. We now describe a procedure to reduce the computational time for the search of Lagrange and Markov edges based on online cycle detection and strongly connected component maintenance \cite{HKMST08, HKMST12, BFGT16}.

Theorem 8. Computing the set of weights of Lagrange edges or the set of weights of Markov edges in a directed weighted graph $G$ can be achieved in $O(m^{3/2})$ where $m$ is the number of edges of $G$.

Proof. Order the edges in $G$ by non-decreasing weight. Namely $E(G) = \{e_1, \ldots, e_m\}$ with $w(e_i) \leq w(e_{i+1})$. We define a sequence of acyclic graphs $(G^{(k)})_{k=0,\ldots,m}$ by identifying the vertices that belong to a same strongly connected component and removing the loops (edges from a vertex to itself). The graph $G^{(k)}$ is concretely obtained from $G^{(k-1)}$ by adding the $k$-th edge and possibly identifying vertices in a newly appeared strongly connected component. As shown in \cite{HKMST08, HKMST12, BFGT16}, maintaining the strongly connected components in dynamical graph, or equivalently computing the sequence $G^{(k)}$, can be done in $O(m^{3/2})$.

Now the weights of Lagrange edges are exactly the weights of edges $e_k$ that create a cycle when they are added in $G^{(k)}$. This shows that it comes at no additional cost. For Markov edges however, one needs to make a further traversal of the graph. However this can be reduced to a total cost of $m$ from which we obtain the same upper bound $O(m^{3/2} + m) = O(m^{3/2})$. In order to do so, one needs to maintain two flags for each edge: whether it can reach in forward and backward directions a non-trivial strongly connected component. Updating these flags is only performed when a new strongly connected component is detected and each edge is at most traversed once.

Now, having this extra information an edge $e_k$ is Markov if and only if at the time it is added in $G^{(k)}$ it is such that its target can reach a strongly connected component in forward direction and its source can reach a strongly connected component in backward direction. □

5. Approximation of Lagrange and Markov spectra

Recall that we defined graphs $G_{K,Q,R}$ in Section 3 and Lagrange and Markov edges in a weighted directed graph were defined in Section 4. The main aim of this section is to prove the following result.

Theorem 9. For any $K,Q$ the set of weights of respectively Lagrange and Markov edges in $G_{K,Q}$ is $1/Q$-close to respectively $L_K$ and $M_K$.

Proof. We do the Markov spectrum, the case of Lagrange being similar.

Let $g \in \Sigma$ and let $m := M(g) = \sup_{n \in \mathbb{Z}} \lambda_0(\sigma^n(g))$. We will show that there is a Markov edge whose weight is $1/Q$-close to $m$. Let $e_0$ be the shift edge corresponding to $\sigma^n(g)$ in the graph $G_{K,Q}$. This sequence of shift edges determine a biinfinite path $\gamma$. Let $e'$ be the edge in $\gamma$ with maximal weight. We claim that $e'$ is a Markov edge of the graph $G_{K,Q}$ and that $|m - F(e')| < 1/Q$.

By construction, we have $|\lambda_0(\sigma^n(g)) - F(e_0)| < 1/Q$. Hence the weight $F(e')$ of the supremum satisfies the required bound. Let $n_0$ be any index such that $e_{n_0} = e'$. Since $\gamma$ is biinfinite, there is a smallest $k$ such that the path $e_{n_0}, e_{n_0+1}, \ldots, e_{n_0+k}$ intersects itself. That is, there is $0 \leq k' < k$ with $e_{n_0+k'} = e_{n_0+k}$. Since the weights on the edges between indices $n_0 + k'$ and $n_0 + k$ are at most $F(e_{n_0})$ we constructed a cycle $\gamma^+$ all of whose weights are at most $F(e_{n_0})$ that can be reached from $e_{n_0}$ by a path with weights not larger than $F(e_{n_0})$. The construction of a path $\gamma^-$ in backward direction is performed similarly and concludes the fact that $e'$ is a Markov edge in $G_{K,Q}$.

\textsuperscript{2}Recall that a directed graph is strongly connected whenever there are oriented paths joining any given pair of vertices and a strongly connected component of a directed graph is a maximal strongly connected directed subgraph.
6. The size of $C_{K,Q}$ and algorithm complexity

As we saw in Section 4, the time complexity of detecting Lagrange and Markov edges in a graph is polynomial in the size of the graph. In this section we provide an upper bound on the size of the graphs $G_{K,Q}$. It will prove the polynomial bounds in Theorem 1.

**Lemma 10.** The number of edges in $G_{K,Q}$ is bounded by

$$|C_{K,Q}| \left( |C_{K,Q}| + \log_2 \left( \frac{(K(K + 1)(K + 2)}{K} \right) \right).$$

To prove the lemma we need to intermediate results that will also be used later. The first one gives a control on the diameter $\text{diam}_K(b)$ in terms of the combinatorial length.

**Lemma 11 (CFS97, Lemma 2 p. 2).** Let $\alpha = [a_0; a_1, \ldots, a_n, a_{n+1}, \ldots]$ and $\beta = [a_0; a_1, \ldots, a_n, b_{n+1}, \ldots]$ with $a_{n+1} \neq b_{n+1}$. Then $|\alpha - \beta| < 1/2^{n-1}$.

The second provides a lower bound on the diameter for edges in $C_{K,Q}$.

**Lemma 12.** For any $Q, K$ and any $\vec{b} \in C_{K,Q}$ we have

$$\frac{K}{(K(K + 1)(K + 2))} \cdot \frac{1}{Q} \leq \text{diam}_K(\vec{b}).$$

**Proof.** On one hand, we have $\frac{\text{diam}_K(\vec{b})}{\text{diam}_K(\vec{b}')}$ for each $\vec{b} \in C_{K, Q}$. On the other hand, we have that

$$(\alpha_K^+ \alpha_K^-)^{-1}(q_n + \alpha_K^- q_{n-1}) < ((K + 1)q_n + q_{n-1}) \leq K(q_n + q_{n-1})$$

and

$$(\alpha_K^+ \alpha_K^-)^{-1}(q_n + \alpha_K^- q_{n-1}) < K(q_n + q_{n-1})$$

Since

$$(\alpha_K^+ \alpha_K^-)^{-1}(q_n + q_{n-1}) = (\alpha_K^+ \alpha_K^-)^{-1}(q_n + q_{n-1})$$

we obtain that

$$\text{diam}_K(\vec{b}) \geq \frac{K}{(K(K + 1)(K + 2))}.$$ 

The estimate follows. □

**Proof of Lemma 11.** Recall that the graph $G_{K,Q}$ has two kind of edges: prolongation edges and shift edges. The shift edges are in bijection with the techniques in [Mor18] and Palis–Takens book [PaTa] to make this relation precise.

Now we need to bound the number of prolongation edges and we claim that there number is at most $Q$. Then

$$\text{diam}_K(\vec{b}) \leq \frac{K}{(K(K + 1)(K + 2))}.$$ 

This follows from Lemma 11 and the lower bound estimates on $\text{diam}_K(\vec{b})$ from Lemma 12. □

It now remains to estimate the size of the sets $C_{K,Q}$. As we will see next, the growth rate in $Q$ is intimately linked to the Hausdorff dimension of the Lagrange and Markov spectra. To do so we apply the techniques in [Mor18] and Palis–Takens book [PaTa] to make this relation precise.

Let us recall that we defined the sets $E_K$ in Section 3 as the image of the one-sided shift $\Sigma^+_K$ under the continued fraction map. More concretely

$$E_K := \{[0; a_1, a_2, \ldots] : a_i \in \{1, \ldots, K\} \subset [0, 1].$$

The set $E_K$ is a closed invariant subset of the Gauss map.

It is known that the Hausdorff dimension $\text{HD}(E_K)$ of $E_K$ is strictly increasing in $K$ and $\text{HD}(E_K) = 1 - \frac{2}{K} - \frac{2}{K^2} + O(1/K^3) \rightarrow 1$ as $K \rightarrow \infty$ (cf. Hensley [He02] and [He96]). For our purposes, it is useful to know that for small values of $K$ we have the following estimates (from [Je04, JePo11, JePo18])

| $K$ | $\text{HD}(E_K)$ |
|-----|-----------------|
| 3   | 0.5312          |
| 4   | 0.7056          |
| 5   | 0.7889          |
Theorem 13. There exist constants \( c_1(K) \) and \( c_2(K) \) such that for any positive integer \( Q \) we have
\[
c_1(K)Q^{\text{HD}(E_K)} \leq |C_{K,Q}| \leq c_2(K)Q^{\text{HD}(E_K)}
\]
where the constants \( c_1(K) \) and \( c_2(K) \) can be explicitly computed.

Putting together the estimates from Lemma 10 and Theorem 13 we obtain an estimate on the size.

Corollary 14. We have \( |G_{K,Q}| = O(Q^{2\text{HD}(E_K)}) \) for \( K = 2, 3, 4 \).

Proof of Theorem 13. Observe that the \( |\vec{b}| \)-th iterate of the Gauss map sends \( I_K(\vec{b}) \) to \([\alpha_K^-, \alpha_K^+]| \). Thus, the average of its derivative \( (\alpha_K^+ - \alpha_K^-)/\text{diam}_K(\vec{b}) \) belong to the interval
\[
(\alpha_K^+ - \alpha_K^-)Q \leq \frac{(\alpha_K^+ - \alpha_K^-)}{\text{diam}_K(\vec{b})} \leq \frac{(\alpha_K^+ - \alpha_K^-)(K(K+1)+1)(K+2)}{K} Q.
\]
Here we used the lower bound estimate from Lemma 12.

Since the distortion of the iterates of the Gauss map (i.e., the ratio between its maximal and minimal derivatives) is \( \leq 4 \) (see, e.g., Proposition 2 in [Mor18]), the maximal derivative \( \Lambda_K(\vec{b}) \) of the \( |\vec{b}| \)-th iterate of the Gauss map on \( I_K(\vec{b}) \) is \( \leq 4(\alpha_K^+ - \alpha_K^-)\frac{(K(K+1)+1)(K+2)}{K} Q \) and the minimal derivative \( \lambda_K(\vec{b}) \) of the \( |\vec{b}| \)-th iterate of the Gauss map on \( I_K(\vec{b}) \) is \( \geq \frac{1}{4}(\alpha_K^+ - \alpha_K^-)Q \).

As it is explained in pages 68 to 70 of Palis–Takens book [PaTa], one has
\[
\sum_{\vec{b} \in C_{K,Q}} \Lambda_K(\vec{b})^{-\text{HD}(E_K)} \leq 1 \leq \sum_{\vec{b} \in C_{K,Q}} \lambda_K(\vec{b})^{-\text{HD}(E_K)}.
\]
In particular, it follows that
\[
c_1(K) := \left( \frac{1}{4}(\alpha_K^+ - \alpha_K^-) \right)^{\text{HD}(E_K)} \leq |C_{K,Q}| \leq \left( 4(\alpha_K^+ - \alpha_K^-)\frac{(K(K+1)+1)(K+2)}{K} \right)^{\text{HD}(E_K)} := c_2(K).
\]
This completes the proof of the desired theorem. \( \square \)
7. Approximation by periodic orbits

In this section we consider the following question. How well the periodic (resp. ultimately periodic) sequences in $\Sigma_K$ with period at most $N$ approximate the set $L_K$ (resp. $M_K$)?

**Proposition 15.** Let $K \in \{2,3,4\}$ and $N \in \mathbb{N}$. Then the subset

$$\bigcup_{k=1}^{2^{4N+1}-1} \{L(\pi) : u \in \{1,\ldots,K\}^k\}$$

is $1/2^{N-2}$-dense in $L_K$. Similarly, the subset

$$\bigcup_{k=1}^{2^{4N+1}-1} \{M(\mu \pi) : \mu \in \{1,2,3,4\}^k\}$$

is $1/2^{N-2}$-dense in $M_4$.

**Proof.** The main ingredient in our estimates is Lemma 11.

**Lagrange spectrum.** Fix $K \in \{2,3,4\}$. Let $\varrho = (a_n)_{n \in \mathbb{Z}} \in \Sigma_K$ and put $t = L(\varrho) \in L$.

By definition, $t = \limsup_{j \to \infty} (\alpha_j + \beta_j)$. Hence, given $\delta > 0$, there are infinitely many $n \in \mathbb{N}$ such that $|\alpha_n + \beta_n - t| < \delta$. Also, there is a sequence $h_m \to +\infty$ as $m \to +\infty$ such that $\alpha_j + \beta_j < t+\delta/m$ for all $j \geq h_m$. Fix $N \in \mathbb{N}$.

Given an index $j$ consider the finite sequence with $2N+1$ terms $(\alpha_{j-N}, \ldots, \alpha_j, \ldots, \alpha_{j+N}) = S(j)$. There is a sequence $S$ such that $S(j) = S$ for infinitely many values of $j$, i.e., there are $j_1 < j_2 < \ldots$ with $S(j_i) = S$, $\forall i \geq 1$. Note that we may (and do) assume that $\lim_{i \to \infty} (\alpha_{j_i} + \beta_{j_i}) = t$.

For each $m \in \mathbb{N}$, consider the subshift of $S$ given by $\Sigma_{t+1/m} = \{\lambda \in \Sigma \mid m(\lambda) \leq t + 1/m\}$. Note that $\Sigma_{t+1/m}$ is invariant by transposition operation $(\lambda_n)_{n \in \mathbb{Z}} \mapsto (\lambda_{-n})_{n \in \mathbb{Z}}$ and by the shift map $\sigma((\lambda_n)_{n \in \mathbb{Z}}) = (\lambda_{n+1})_{n \in \mathbb{Z}}$. Moreover, it is contained (and well approximated) by the following subshift of finite type: let $\tilde{B}$ be the set of all factors of size $2N+1$ of all elements of $\Sigma_{t+1/m}$, and denote by $\tilde{\Sigma}_{t+1/m,N}$ the set of all infinite words in $\Sigma$ whose factors of size $2N+1$ are all in $B$.

We can describe $\tilde{\Sigma}_{t+1/m,N}$ as a (not necessarily transitive) Markov shift: the allowed transitions are of the type $(c_0, c_1, c_2, \ldots, c_{2N+1})$ with $(c_0, c_1, \ldots, c_{2N})$ and $(c_1, c_2, \ldots, c_{2N+1})$ belonging to $B$.

By definition, we have $S \in B$, and it is possible to connect $S$ to itself in $\tilde{\Sigma}_{t+1/m,N}$ by a sequence of allowed transitions. The minimum number $k$ of transitions needed to connect $S$ to itself in $\tilde{\Sigma}_{t+1/m,N}$ is trivially bounded by the size of $B$, which is at most $K^{2N+1}$.

In other words, for each $m \in \mathbb{N}$, there is $1 \leq k \leq K^{2N+1}$ and a factor $\omega_m = (\tilde{a}_0, \tilde{a}_1, \ldots, \tilde{a}_{2N+k})$ of size $2N+k+1$ of an element of $\tilde{\Sigma}_{t+1/m,N}$ with $(\tilde{a}_0, \ldots, \tilde{a}_{2N}) = S$.

In particular, if $\tilde{\theta}_m = (\tilde{a}_0, \ldots, \tilde{a}_{k-1})$ is the periodic sequence of period $\tilde{a}_0 \ldots \tilde{a}_{k-1}$, then Lemma 11 ensures that $|L(\tilde{\theta}_m) - t| < 1/m + 2/2^{2N+1}$. Since $k \leq K^{2N+1}$, there is a periodic sequence $\tilde{\pi}$ with period $\leq K^{2N+1}$ such that $\tilde{\pi} = \tilde{\theta}_m$ for infinitely many $m \in \mathbb{N}$ and, a fortiori, $|L(\tilde{\pi}) - t| \leq 2/2^{2N+1}$.

**Markov spectrum.** Let $\tilde{\varrho} = (b_n)_{n \in \mathbb{Z}} \in \Sigma$, consider $s = m(\tilde{\varrho}) \in L$, and suppose that $b_n = 4$ for all $n \in \mathbb{Z}$. We may (and do) also assume that $s = a_0 + \beta_0$.

By the pigeonhole principle, there are $1 \leq i < j \leq 4^{2N+1}+1$ and $1 \leq u < v \leq 4^{2N+1}+1$ such that $(b_i, b_{i+1}, \ldots, b_{i+2N}) = (b_j, b_{j+1}, \ldots, b_{j+2N})$ and $(b_{u-1}, b_{u-2}, \ldots, b_{u-2N}) = (b_{v-1}, b_{v-2}, \ldots, b_{v-2N})$.

By Lemma 11 if $\tilde{\varrho}$ is the doubly pre-periodic sequence

$$(b_{v-1}, b_{v-2}, \ldots, b_{u-2}, b_{u-1})b_{u-1} \ldots b_{i-1}(b_i, b_{i+1}, \ldots, b_{j-1})$$

then $|m(\tilde{\varrho}) - s| < 2/2^{2N-1}$. Notice that the total size of the block formed by the central block and the periods on both sides is at most $2 \cdot 4^{2N+1} - 1$.

**Remark 16.** The Markov spectrum $M$ is also characterized by the values of real indefinite binary quadratic forms (see [CF89, Chapter 1]). An attempt to draw some portions of $M$ using certain binary quadratic forms of bounded heights was performed by T. Morrison [Mo12], but unfortunately this text does not discuss the quality of the approximation of $M$ obtained by this method.
8. High resolution Lagrange spectra $L_2$ and $L_3$

Figure 5. Pictures of Lagrange spectra $L_2$ and $L_3$ obtained from our algorithm. The parameters $Q_2$ and $Q_3$ are so that the Lagrange spectra $L_2$ and $L_3$ are respectively at most at Hausdorff distance $1/Q_2$ and $1/Q_3$ from the union of blue intervals.
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