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 α we define the *best constant of Diophantine approximation of* α as

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

where p and q are bound to be positive integers. The *Lagrange spectrum* $\mathbf{L}$ is the set $\{\mathrm{L}(\alpha) : \alpha \in \mathbb{R} \setminus \mathbb{Q}\}$. Perron [Per21] showed that if $\alpha = [a_0; a_1, \ldots]$ is the continued fraction expansion of α, then

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

In other words, one can equivalently define the Lagrange spectrum on the biinfinite 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

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

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

$$\mathbf{M} = \{\mathrm{M}(\underline{a}) : \underline{a} \in \Sigma\},$$

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

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

$$0.53128 < \mathrm{HD}(\mathbf{M} \setminus \mathbf{L}) < 0.986927.$$

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Also, it was shown by Freiman [Fre73] and Schecker [Sch77] that $\mathbf{L}$ contains the half-line $[\sqrt{21}, +\infty)$. We recommend consulting Cusick–Flahive's 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 $\mathbf{L}$ and $\mathbf{M}$ 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 sets of real numbers. We say that X and Y are ε-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 provides 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 $R \leq \sqrt{13} \sim 3.606$,*
- *$d_R < 0.706$ for $R \leq 2\sqrt{5} \sim 4.472$,*
- *$d_R < 0.789$ for $R \leq \sqrt{21} \sim 4.583$.*

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 contain only the digits from 1 to K.

Remark 2. As we mentioned already, $\mathbf{L}$ 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 $\mathbf{L}$ and $\mathbf{M}$ could potentially lead the way to solving some long-standing questions such as Berstein's[1] conjecture [Be73] that $[4.1, 4.52] \subset \mathbf{L}$. 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 $\mathbf{L}_K$ and $\mathbf{M}_K$, respectively, the Lagrange and Markov spectra restricted to the shift Σ_K, that is, $\mathbf{L}_K = \{\mathrm{L}(\underline{a}) : \underline{a} \in \Sigma_K\}$ and $\mathbf{M}_K = \{\mathrm{M}(\underline{a}) : \underline{a} \in \Sigma_K\}$. For each K, the relation $\mathbf{L}_K \subset \mathbf{M}_K$ holds.

The first step of the algorithm consists of 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

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

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[1] In fact, despite the fact that some heuristic arguments from the projection theory of fractal sets are compatible with the presence of intervals in $\mathbf{L}$ before the so-called Hall's ray, Berstein's conjecture is somewhat surprising to us because it proposes a concrete *relatively large* interval before Hall's ray.

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

We turn the graph $G_{K,Q}$ into a weighted graph by considering on the edge associated to $\vec{b}$ the weight $\frac{\inf_{\underline{a} \in \vec{b}} \lambda_0(\underline{a}) + \sup_{\underline{a} \in \vec{b}} \lambda_0(\underline{a})}{2}$. The weighted graph $G_{K,Q}$ provides an approximation of the shift Σ_K together with the height function λ_0. The condition (1) gives the upper bound on the quality of approximation. The rest of the algorithm consists of studying directly on the graph $G_{K,Q}$ the discrete analogue of Lagrange and Markov spectra. The overall complexity of the algorithm is governed by the size of $G_{K,Q}$. It is not so suprising 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 $\mathbf{L}_K$ for $1 \leq K \leq 4$. In Section 3, we describe the weighted directed graphs $G_{K,Q}$ and their basic properties. After that, Section 4 provides the discrete analogue of Lagrange and Markov spectra on a weighted directed graph. In Section 5, we justify that the discrete spectra 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^4} periodic orbits in order to rigorously ensure that we get a $(1/Q)$-dense subset of $\mathbf{L}$!

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

2. Preliminary bounds on $\mathbf{L}_K$

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

The points

$$[0; \overline{1}] = \frac{\sqrt{5}-1}{2} \qquad [0; \overline{2}] = \sqrt{2}-1 \qquad [0; \overline{3}] = \frac{\sqrt{13}-3}{2} \qquad [0; \overline{4}] = \sqrt{5}-2$$
$$\simeq 0.6180 \qquad\qquad \simeq 0.4142 \qquad\qquad \simeq 0.3028 \qquad\qquad \simeq 0.2361$$

and

$$[0; \overline{2,1}] = \frac{\sqrt{3}-1}{2} \qquad\qquad [0; \overline{3,1}] = \frac{\sqrt{21}-3}{6} \qquad\qquad [0; \overline{4,1}] = \frac{\sqrt{2}-1}{2}$$
$$\simeq 0.3660 \qquad\qquad\qquad \simeq 0.2638 \qquad\qquad\qquad \simeq 0.2071$$

$$[0; \overline{1,2}] = \sqrt{3}-1 \qquad\qquad [0; \overline{1,3}] = \frac{\sqrt{21}-3}{2} \qquad\qquad [0; \overline{1,4}] = 2\sqrt{2}-2$$
$$\simeq 0.7321 \qquad\qquad\qquad \simeq 0.7913 \qquad\qquad\qquad \simeq 0.8284$$

allow us to determine the intervals containing $\mathbf{L}_K \setminus \mathbf{L}_{K-1}$ for $1 \leq K \leq 4$; see Figure 1.
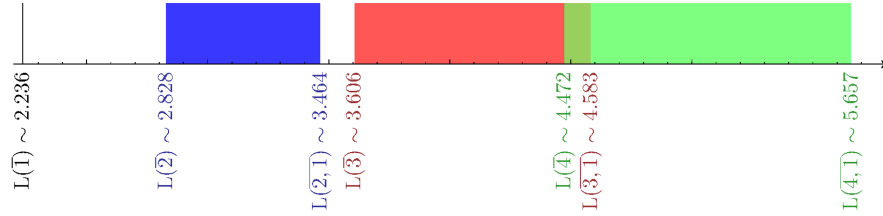

FIGURE 1. The lower and upper bounds for $\mathbf{L}_K \setminus \mathbf{L}_{K-1}$ when $1 \leq K \leq 4$.

The ranges of R for which we provide upper bounds on d_R in Theorem 1 are visible on Figure 1:

- $\mathrm{L}(\overline{2,1}) = \sqrt{13}$ is the maximum of $\mathbf{L}_2$.
- $\mathrm{L}(\overline{4}) = 2\sqrt{5}$ is the maximum of $\mathbf{L}_4 \setminus \mathbf{L}_3$.

Let us also mention that $\mathrm{L}(\overline{3,1}) = \sqrt{21}$ is the maximum of $\mathbf{L}_3$.

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 $G_{K,Q}^+$ that are associated to the one-sided shift $\Sigma_K^+ := \{1, \ldots, K\}^{\mathbb{N}}$.

3.1. $(1/Q)$-cylinders for the Gauss map.

In this section we consider approximations of Σ_K^+ by shift of finite type. The continued fraction embeds the shift Σ_K^+ into $\mathbb{R}$ as

$$\begin{array}{ccc} \Sigma_K^+ & \to & \mathbb{R}_+ \\ \underline{a} = (a_n)_{n\geq 1} & \mapsto & [0; a_1, a_2, \ldots]. \end{array}$$

The image of Σ_K^+ under this map is a Cantor set E_K.

For a finite (one-sided) cylinder $\vec{b} = (b_1, \ldots, b_n)$ for the Gauss map we use the notation

$$\frac{p_k(\vec{b})}{q_k(\vec{b})} = \cfrac{1}{b_1 + \cfrac{1}{b_2 + \cdots + \cfrac{1}{b_k}}}.$$

A cylinder $\vec{b} \in \{1, \ldots, K\}^n$ projects on $[0,1]$ on a subset $I_K(\vec{b}) \cap E_K$ where $I_K(\vec{b})$ is the interval with extremities

$$\frac{p_n(\vec{b}) + \alpha_K^+ \, p_{n-1}(\vec{b})}{q_n(\vec{b}) + \alpha_K^+ \, q_{n-1}(\vec{b})} \quad \text{and} \quad \frac{p_n(\vec{b}) + \alpha_K^- \, p_{n-1}(\vec{b})}{q_n(\vec{b}) + \alpha_K^- \, q_{n-1}(\vec{b})},$$

where $\alpha_K^- = [0; \overline{K, 1}]$ and $\alpha_K^+ = [0; \overline{1, K}]$. The values of α_K^- and α_K^+ for $K \in \{1, 2, 3, 4\}$ were computed in Section 2. Note that depending on the parity of the length $|\vec{b}|$ of $\vec{b}$ one or the other is the left-hand side of the interval. The diameter of $I_K(\vec{b})$ is

(2) $$\operatorname{diam}_K(\vec{b}) := \frac{(\alpha_K^+ - \alpha_K^-)}{(q_n(\vec{b}) + \alpha_K^+ \, q_{n-1}(\vec{b}))(q_n(\vec{b}) + \alpha_K^- \, q_{n-1}(\vec{b}))}.$$

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

(3) $$C_{K,Q} := \left\{ \vec{b} \in \{1, \ldots, K\}^+ : \ \operatorname{diam}_K(\vec{b}) \leq \frac{1}{Q} < \operatorname{diam}_K(\vec{b}') \right\},$$

where $\vec{b}'$ denotes the prefix of length $|\vec{b}| - 1$ of b and diam_K 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 of as the leaves of a tree rooted at the empty word ε 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 set $\overline{C}_{K,Q}$, 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.

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 an edge a *prolongation edge* (they are in black on Figure 2). Second, 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 u that avoids any other element from $V_{K,Q}^+$. We add an edge from w to v that we call a *shift edge*.
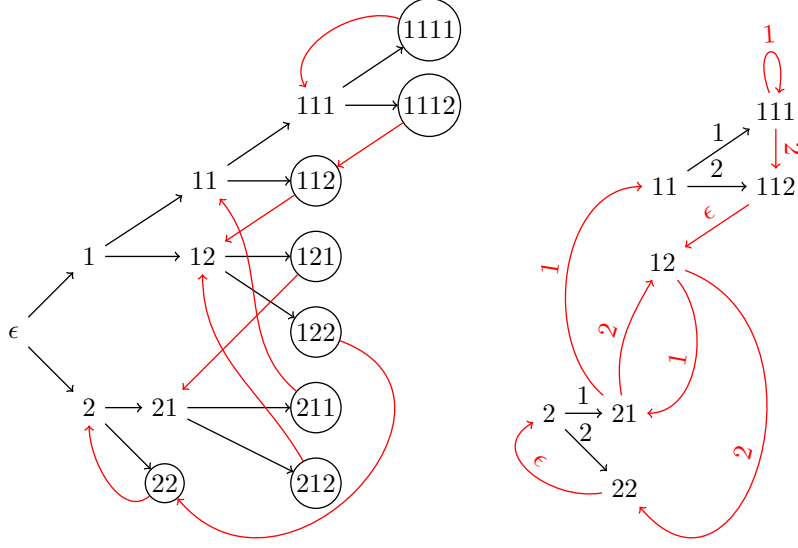
FIGURE 2. The tree of $T_{2,20}$ and the suffix links (in red) on the left. The graph $G_{2,20}^+$ on the right with the prolongation edges in black and the shift edges in red.

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 carries 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 $G_{K,Q}^+$ recognizes the shift $\{1, \ldots, K\}^{\mathbb{Z}}$: for any biinfinite word $w \in \Sigma_K$ there exists a unique biinfinite path γ in $G_{K,Q}^+$ so that w can be read along γ.*

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 Σ_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 obtained the de Bruijn graph [dBr].

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 $0 \le k \le n$. 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

$$(4) \qquad F((p, a_0, s)) = a_0 + \mathrm{mid}_K(p) + \mathrm{mid}_K(s),$$

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

$$(5) \qquad \mathrm{mid}_K(\vec{b}) = \frac{1}{2} \left(\frac{p_n(\vec{b}) + \alpha_K^+ \, p_{n-1}(\vec{b})}{q_n(\vec{b}) + \alpha_K^+ \, q_{n-1}(\vec{b})} + \frac{p_n(\vec{b}) + \alpha_K^- \, p_{n-1}(\vec{b})}{q_n(\vec{b}) + \alpha_K^- \, q_{n-1}(\vec{b})} \right).$$

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 Σ_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*

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

Proof. Recall that the weights defined in (4) are in between the extremal possible values of $\lambda_0(\underline{a})$ in the cylinder (p, a_0, s). But p and s are in $C_{K,Q}$ constructed in Section 3.1 and were chosen so that the corresponding image under the continued fraction map has diameter $< 1/Q$. Hence for each of $\mathrm{mid}_K(p)$ and $\mathrm{mid}_K(s)$ we are off by at most $1/(2Q)$ so that $a_0 + \mathrm{mid}_K(p) + \mathrm{mid}_K(s)$ is off by at most $1/Q$. $\quad\square$

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

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

4. Lagrange and Markov edges in weighted directed graphs

Let G be a weighted directed graph. We denote by $V(G)$ 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 need not be $\mathbb{R}$; any totally ordered set would do.

We call an edge e in G a *Lagrange edge* if there exists a cycle γ in G that passes through e and so that the weight of the edge e is maximal among the weights of edges in γ. An edge is called a *Markov edge* if there exist two cycles γ^- and γ^+ and a path p from γ^- to γ^+ 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.

A simple approach for computing these edges is to test for each edge whether it is Lagrange or Markov.
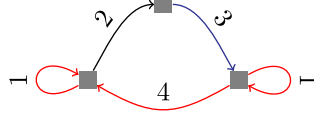
FIGURE 3. A weighted graph with its Lagrange edges in red and its single Markov but not Lagrange edge in blue.

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 let u and v be 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 [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 considering the graph obtained from the edges $\{e_1, \ldots, e_k\}$, identifying the vertices that belong to a same strongly connected component[2] 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 [HKMST08, HKMST12, BFGT16], maintaining the strongly connected components in a 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 performed only when a new strongly connected component is detected and each edge is at most traversed once.

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[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.

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, $\mathbf{L}_K$ and $\mathbf{M}_K$.*

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

Let $\underline{a} \in \Sigma$ and let $m := \mathrm{M}(\underline{a}) = \sup_{n \in \mathbb{Z}} \lambda_0(\sigma^n(\underline{a}))$. We will show that there is a Markov edge whose weight is $1/Q$-close to m. Let e_n be the shift edge corresponding to $\sigma^n(\underline{a})$ in the graph $G_{K,Q}$. This sequence of shift edges determines a biinfinite path γ. Let e' be the edge in γ 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 $|\lambda_0(\sigma^n(\underline{a})) - F(e_n)| < 1/Q$. 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 γ 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 $0 \le k' < k$ 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 γ^+ 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 γ^- in backward direction is performed similarly and concludes the fact that e' is a Markov edge in $G_{K,Q}$. □

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*

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

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

Lemma 11 ([CF89, Lemma 2, p. 2]). *Let $\alpha = [a_0; a_1, \ldots, a_n, a_{n+1}, \ldots]$ and let $\beta = [a_0; a_1, \ldots, a_n, b_{n+1}, \ldots]$ with $a_{n+1} \ne b_{n+1}$. Then $|\alpha - \beta| < 1/2^{n-1}$.*

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

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

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

Proof. On one hand, we have $\frac{\operatorname{diam}_K(\vec{b})}{\operatorname{diam}_K(\vec{b}')} = \frac{(q_{n-1}+\alpha_K^+ q_{n-2})(q_{n-1}+\alpha_K^- q_{n-2})}{(q_n+\alpha_K^+ q_{n-1})(q_n+\alpha_K^- q_{n-1})}$ for each $\vec{b} \in C_{K,Q}$. On the other hand, we have that

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

and

$$(\alpha_K^+ \alpha_K^-)^{-1}(q_{n-1} + \alpha_K^+ q_{n-2})(q_{n-1} + \alpha_K^- q_{n-2}) > (Kq_{n-1} + q_{n-2})(q_{n-1} + q_{n-2}).$$

Since

$$(\tfrac{K+1}{K}q_n + q_{n-1}) = (\tfrac{K+1}{K}a_n q_{n-1} + \tfrac{K+1}{K}q_{n-2} + q_{n-1}) \leq (K+2)(q_{n-1} + q_{n-2})$$

and

$$((K+1)q_n + q_{n-1}) = ((K+1)a_n q_{n-1} + (K+1)q_{n-2} + q_{n-1}) \leq \tfrac{(K+1)K+1}{K}(Kq_{n-1} + q_{n-2}),$$

we obtain that

$$\frac{\operatorname{diam}_K(\vec{b})}{\operatorname{diam}_K(\vec{b}')} > \frac{K}{(K(K+1)+1)(K+2)}.$$

The estimate follows. □

Proof of Lemma 10. Recall that the graph $G_{K,Q}$ has two kinds of edges: prolongation edges and shift edges. The shift edges are in bijection with $C_{K,Q} \times C_{K,Q}$, which provides the term in $|C_{K,Q}|^2$.

Now we need to bound the number of prolongation edges and we claim that the number is at most

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

This follows from Lemma 11 and the lower bound estimates on $\operatorname{diam}_K(\vec{b})$ 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's 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 Σ_K^+ under the continued fraction map. More concretely

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

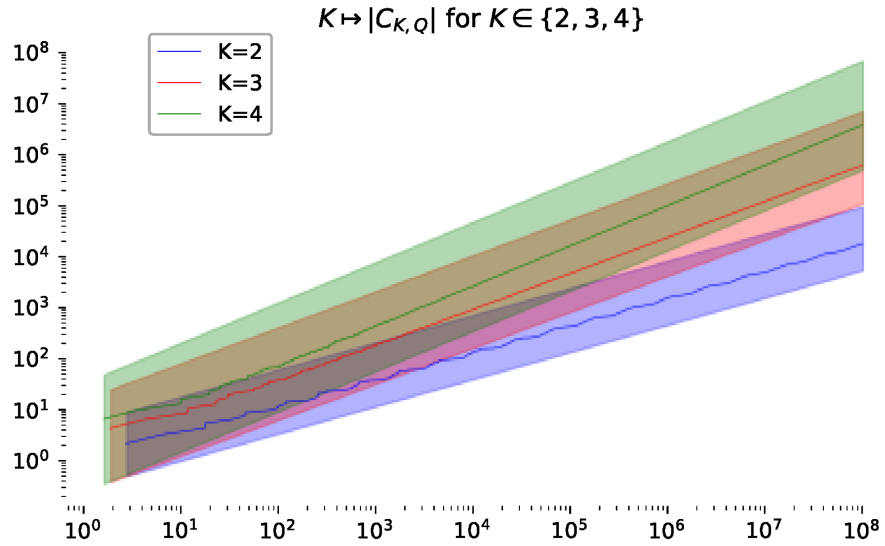The set E_K is a closed invariant subset of the Gauss map.

FIGURE 4. Sizes of the set $C_{K,Q}$ in log scale. The lighter color represents the bound we obtain from Theorem 13 together with the estimates on $\mathrm{HD}(E_K)$ (from $[\mathrm{Je}04, \mathrm{JePo}01, \mathrm{JePo}18]$).

It is known that the Hausdorff dimension $\mathrm{HD}(E_K)$ of E_K is strictly increasing in K and $\mathrm{HD}(E_K) = 1 - \frac{6}{\pi^2}K - \frac{72}{\pi^4}\frac{\log K}{K^2} + O(1/K^2) \to 1$ as $K \to \infty$ (cf. Hensley $[\mathrm{He}92]$ and $[\mathrm{He}96]$). For our purposes, it is useful to know that for small values of K we have the following estimates (from $[\mathrm{Je}04, \mathrm{JePo}01, \mathrm{JePo}18]$):

$$0.5312 < \mathrm{HD}(E_2) < 0.5313,$$
$$0.7056 < \mathrm{HD}(E_3) < 0.7057,$$
$$0.7889 < \mathrm{HD}(E_4) < 0.7890.$$

Theorem 13. *There exist constants $c_1(K)$ and $c_2(K)$ such that for any positive integer Q we have*

$$c_1(K)Q^{\mathrm{HD}(E_K)} \leq |C_{K,Q}| \leq c_2(K)Q^{\mathrm{HD}(E_K)},$$

where the constants $c_1(K)$ and $c_2(K)$ can be explicitly computed:

K	$c_1(K)$	$c_2(K)$,
2	0.28	4.98,
3	0.23	14.85,
4	0.23	31.2.

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

Corollary 14. *We have $|G_{K,Q}| = O(Q^{2\,\mathrm{HD}(E_K)})$ 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 $(\alpha_K^+ - \alpha_K^-)/\operatorname{diam}_K(\vec{b})$ belongs to the interval

$$(\alpha_K^+ - \alpha_K^-)Q \leq \frac{(\alpha_K^+ - \alpha_K^-)}{\operatorname{diam}_K(\vec{b})} \leq (\alpha_K^+ - \alpha_K^-)\frac{(K(K+1)+1)(K+2)}{K}Q.$$

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 ≤ 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 is explained on pages 68 to 70 of Palis–Takens's book [PaTa], one has

$$\sum_{\vec{b} \in C_{K,Q}} \Lambda_K(\vec{b})^{-\operatorname{HD}(E_K)} \leq 1 \leq \sum_{\vec{b} \in C_{K,Q}} \lambda_K(\vec{b})^{-\operatorname{HD}(E_K)}.$$

In particular, it follows that

$$c_1(K) := \left(\frac{1}{4}(\alpha_K^+ - \alpha_K^-)\right)^{\operatorname{HD}(E_K)} \leq \frac{|C_{K,Q}|}{Q^{\operatorname{HD}(E_K)}}$$

$$\leq \left(4(\alpha_K^+ - \alpha_K^-)\frac{(K(K+1)+1)(K+2)}{K}\right)^{\operatorname{HD}(E_K)} := c_2(K).$$

This completes the proof of the desired theorem. $\qquad\square$

7. APPROXIMATION BY PERIODIC ORBITS

In this section we consider the following question. How well do the periodic (resp., ultimately periodic) sequences in Σ_K with period at most N approximate the set $\mathbf{L}_K$ (resp., $\mathbf{M}_K$)?

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

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

is $1/2^{N-2}$-dense in $\mathbf{L}_K$. Similarly, the subset

$$\bigcup_{k=1}^{2 \cdot 4^{2N+1}-1} \{\mathrm{M}(\overline{p}\,u\,\overline{s}) : pus \in \{1, 2, 3, 4\}^k\}$$

is $1/2^{N-2}$-dense in $\mathbf{M}_4$.

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

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

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 $\alpha_j + \beta_j < t + 1/m$ for all $j \geq h_m$. Fix $N \in \mathbb{N}$. Given an index j consider the finite sequence with $2N + 1$ terms $(a_{j-N}, \ldots, a_j, \ldots, a_{j+N}) =: S(j)$. There is a sequence S such that $S(j) = S$ for infinitely many values of j; i.e., there are $j_1 < j_2 < \cdots$ 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 Σ given by $\Sigma_{t+1/m} = \{\underline{\lambda} \in \Sigma \mid m(\underline{\lambda}) \leq t + 1/m\}$. 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 B be the set of all factors of size $2N + 1$ of all elements of $\Sigma_{t+1/m}$, and denote by $\widetilde{\Sigma}_{t+1/m,N}$ the set of all infinite words in Σ whose factors of size $2N + 1$ are all in B.

We can describe $\widetilde{\Sigma}_{t+1/m,N}$ as a (not necessarily transitive) Markov shift: the allowed transitions are of the type $(c_0, c_1, c_2, \ldots, c_{2N}, c_{2N+1})$ 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 $\widetilde{\Sigma}_{t+1/m,N}$ by a sequence of allowed transitions. The minimum number k of transitions needed to connect S to itself in $\widetilde{\Sigma}_{t+1/m,N}$ 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 $\widetilde{\Sigma}_{t+1/m,N}$ with $(\tilde{a}_0, \ldots, \tilde{a}_{2N}) = (\tilde{a}_k, \ldots, \tilde{a}_{2N+k}) = S$. In particular, if $\tilde{\theta}_m = \overline{(\tilde{a}_0, \ldots, \tilde{a}_{k-1})}$ is the periodic sequence of period $\tilde{a}_0 \cdots \tilde{a}_{k-1}$, then Lemma 11 ensures that $|\mathrm{L}(\tilde{\theta}_m) - t| < 1/m + 2/2^{N-1}$. Since $k \leq K^{2N+1}$, there is a periodic sequence $\overline{\mu}$ with period $\leq K^{2N+1}$ such that $\overline{\mu} = \tilde{\theta}_m$ for infinitely many $m \in \mathbb{N}$ and, a fortiori, $|\mathrm{L}(\overline{\mu}) - t| \leq 2/2^{N-1}$.

Markov spectrum. Let $\underline{\theta} = (b_n)_{n \in \mathbb{Z}} \in \Sigma$, consider $s = m(\underline{\theta}) \in L$, and suppose that $b_n \leq 4$ for all $n \in \mathbb{Z}$. We may (and do) also assume that $s = \alpha_0 + \beta_0$.

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

By Lemma 11, if $\hat{\theta}$ is the doubly pre-periodic sequence

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

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

Remark 16. The Markov spectrum $\mathbf{M}$ is also characterized by the values of real indefinite binary quadratic forms (see [CF89, Chapter 1]). An attempt to draw some portions of $\mathbf{M}$ 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 $\mathbf{M}$ obtained by this method.
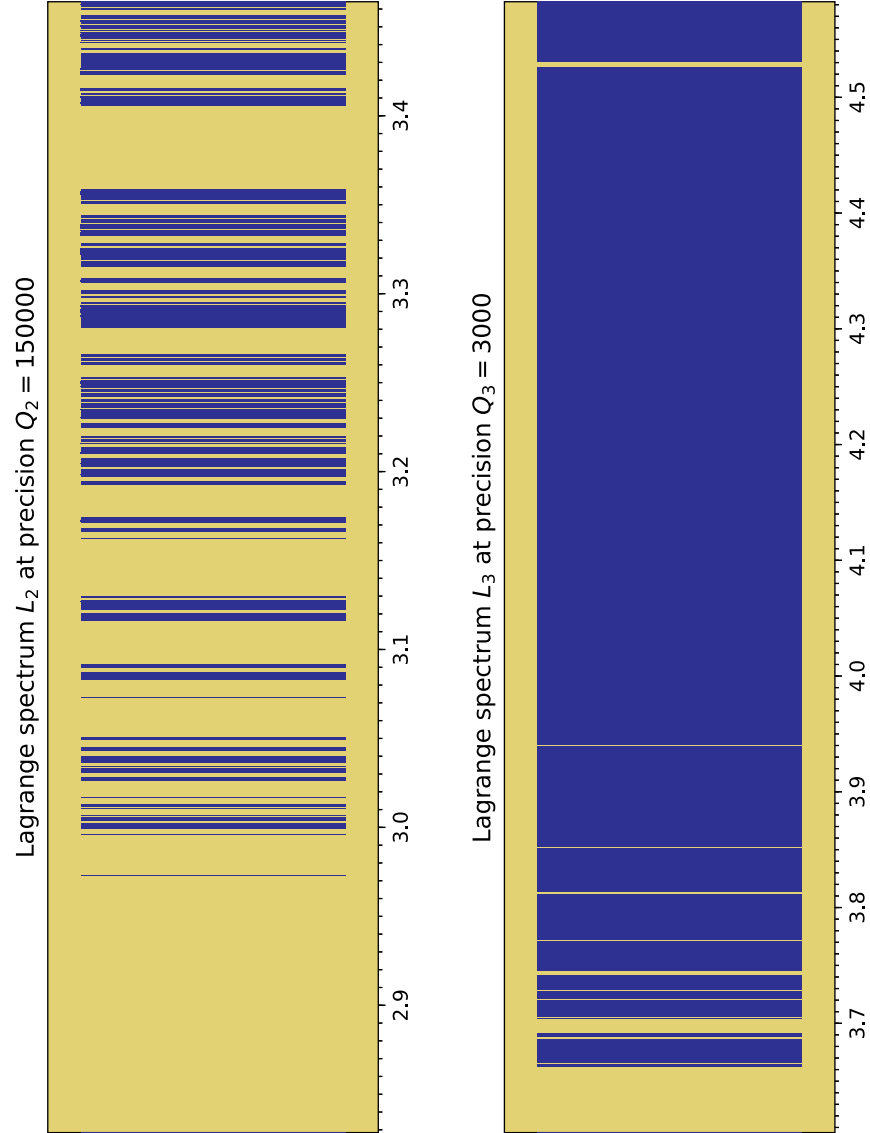
8. High resolution Lagrange spectra $\mathbf{L}_2$ and $\mathbf{L}_3$

FIGURE 5. Pictures of Lagrange spectra $\mathbf{L}_2$ and $\mathbf{L}_3$ obtained from our algorithm. The parameters Q_2 and Q_3 are so that the Lagrange spectra $\mathbf{L}_2$ and $\mathbf{L}_3$ are, respectively, at most at Hausdorff distance $1/Q_2$ and $1/Q_3$ from the union of blue intervals.

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