THE PSLQ ALGORITHM FOR EMPIRICAL DATA

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Abstract. The celebrated integer relation finding algorithm PSLQ has been successfully used in many applications. However, the PSLQ was only analyzed theoretically for exact input. When the input data are irrational numbers, they must be approximate ones due to finite precision in computer. That is, when the algorithm takes empirical data (inexact data with error bounded) instead of exact real numbers as its input, how do we ensure theoretically the output of the algorithm to be an exact integer relation? In this paper, we investigate the PSLQ algorithm for empirical data as its input. First, we give a termination condition for this case. Secondly, we analyze a perturbation on the hyperplane matrix constructed from the input data and hence disclose a relationship between the accuracy of the input data and the output quality (an upper bound on the absolute value of the inner product of the exact data and the computed integer relation). Further, we also analyze the computational complexity for PSLQ with empirical data. Examples on transcendental numbers and algebraic numbers show the meaningfulness of our error control strategies.

1. Introduction

A vector \( m \in \mathbb{Z}^n \setminus \{0\} \) is called an integer relation for \( \alpha \in \mathbb{R}^n \) if \( \langle \alpha, m \rangle = 0 \). The problem of finding integer relations for rational or real numbers can be dated back to the time of Euclid. It is closely related to the problem of finding a small vector in a Euclidean lattice. In fact, the celebrated Lenstra-Lenstra-Lovász (LLL) lattice basis reduction algorithm can be used to find an integer relation. This was already pointed out in [15, page 525]. The HJLS algorithm [11] is the first proved polynomial time algorithm for integer relation finding. The PSLQ algorithm [8, 9] is one of the most frequently used algorithms to find integer relations. Both HJLS and PSLQ can be viewed as algorithms to compute the intersection between a lattice and a vector space; see [7]. For detailed historical notes, we refer to [11, 9]. Nowadays, integer relation finding has been successfully used in different areas, such as experimental math [5, 17] and physics [4]. For more applications, we refer to [6] and the references therein.

However, there always exist some data that can only be obtained with limited accuracy. Indeed, all the input data in applications above are of limited accuracy, and hence not exact values. Consequently, it is of great importance to study how...
to compute an exact integer relation of \( \alpha \) from the approximate input data \( \bar{\alpha} \) by PSLQ.

To the best of our knowledge, there exists only an experienced result on this topic, due to Bailey [2]. Bailey in [2] suggested that if one wishes to recover an integer relation with coefficients bounded by \( G \) for an \( n \)-dimensional vector \( \alpha \), then the input vector \( \alpha \) must be specified to at least \( n \log_{10} G \) decimal digits, and one must employ floating-point arithmetic with at least \( n \log_{10} G \) accurate digits. Bailey’s suggestion works well in practice, however lacks theoretical support. In this paper, we attempt to provide a theory for the error control of PSLQ.

Let \( \alpha = (\alpha_1, \ldots, \alpha_n) \in \mathbb{R}^n \) be the intrinsic data (exact data that may not be known) with an integer relation within a 2-norm bound \( M \), and \( \bar{\alpha} \) be the empirical data with \( \|\alpha - \bar{\alpha}\|_2 < \varepsilon_1 \). Generally, \( \bar{\alpha} \) may not have an integer relation within the bound \( M \). Therefore, the algorithm of PSLQ may not terminate when we compute an integer relation from \( \bar{\alpha} \) by PSLQ because the element \( h_{n,n-1} \) of the hyperplane matrix (see Definition 2.1 and Algorithm 4) may never be transformed to zero.

So, firstly, we need to reconsider the termination condition of PSLQ. Secondly, even if we obtain certain \( m \) from \( \bar{\alpha} \), we need to determine whether \( \langle \alpha, m \rangle = 0 \), without knowing the intrinsic data \( \alpha \). To do this requires a gap bound \( \delta \) for \( \|\alpha, m\| \). A so-called gap bound for \( \|\alpha, m\| \) is that there exist a given \( \delta > 0 \) such that \( \|\alpha, m\| > \delta \) whenever \( \|\alpha, m\| \neq 0 \). If there exists no further information about \( \alpha \), then there does not exist a gap bound in general. However, a gap bound can be given when \( \alpha_i \)'s are algebraic numbers [14, 13]. Once we have a gap bound \( \delta \) and \( \|\alpha, m\| < \delta \), it guarantees \( \langle \alpha, m \rangle = 0 \), even without knowing \( \alpha \). In this paper, we will not discuss the gap bound, but focus on how to estimate \( \|\alpha, m\| \) from its approximation \( \bar{\alpha} \) by establishing a relation between \( \|\alpha, m\| \) and \( \|\alpha, m\| \).

Thirdly, we analyze the computation complexity for PSLQ with empirical data. Finally, we also give some illustrative examples that show how helpful the error control strategies are for applications of PSLQ.

2. Preliminaries

For completeness, we recall the PSLQ algorithm in this section. As indicated in [9], PSLQ works for both of the real case and the complex case. For the complex case, it may find a Gaussian integer relation for a given \( \alpha \in \mathbb{C}^n \). For simplicity, we only consider the real case here.

Let \( \alpha = (\alpha_1, \ldots, \alpha_n) \in \mathbb{R}^n \) with \( \alpha_i \neq 0 \) for \( i = 1, \ldots, n \).

**Definition 2.1 (Hyperplane matrix).** Given \( \alpha \) as above, define the hyperplane matrix \( H_\alpha \) as

\[
H_\alpha = \frac{\alpha}{\bar{\alpha}} = \begin{pmatrix}
\frac{\alpha_1}{h_{n,n-1}} & \frac{\alpha_2}{h_{n,n-1}} & \frac{\alpha_3}{h_{n,n-1}} & \cdots & \frac{\alpha_n}{h_{n,n-1}} \\
\frac{\bar{\alpha}_1}{\bar{\alpha}_1} & \frac{\bar{\alpha}_2}{\bar{\alpha}_2} & \frac{\bar{\alpha}_3}{\bar{\alpha}_3} & \cdots & \frac{\bar{\alpha}_n}{\bar{\alpha}_n} \\
\frac{\bar{\alpha}_1}{\bar{\alpha}_1} & \frac{\bar{\alpha}_2}{\bar{\alpha}_2} & \frac{\bar{\alpha}_3}{\bar{\alpha}_3} & \cdots & \frac{\bar{\alpha}_n}{\bar{\alpha}_n} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
\frac{\bar{\alpha}_1}{\bar{\alpha}_1} & \frac{\bar{\alpha}_2}{\bar{\alpha}_2} & \frac{\bar{\alpha}_3}{\bar{\alpha}_3} & \cdots & \frac{\bar{\alpha}_n}{\bar{\alpha}_n}
\end{pmatrix},
\]

where \( s_j^2 = \sum_{k=j}^n \alpha_k^2 \).
Further, we can assume that \( \|\alpha\|_2 = 1 \), since the hyperplane matrix \( H_\alpha \) is scale-invariant with respect to \( \alpha \), i.e., \( H_\alpha = H_{c,\alpha} \) for \( c \in \mathbb{R} \setminus \{0\} \).

Algebraically, PSLQ produces a series of unimodular matrices in \( \text{GL}_n(\mathbb{Z}) \) acting \( H_\alpha \) from left and a series of orthogonal matrices from right. These matrices are produced by the following subroutines (Algorithm 1, 2 and 3).

**Algorithm 1** (SizeReduction)

**Input:** A lower trapezoidal \( n \times (n-1) \) matrix \( H = (h_{i,j}) \) with \( h_{i,j} = 0 \) if \( j > i \) and \( h_{j,j} \neq 0 \).

**Output:** A unimodular matrix \( D \) such that \( H := D \cdot H = (h_{i,j}) \) satisfying \( |h_{i,j}| \leq |h_{j,j}|/2 \) for \( 1 \leq j < i \leq n \).

1: \( D := I_n \).
2: for \( i \) from 2 to \( n \) do
3:   for \( j \) from \( i - 1 \) to 1 by stepsize \(-1\) do
4:     \( q := \lfloor h_{i,j}/h_{j,j} + 0.5 \rfloor \).
5:     for \( k \) from 1 to \( n \) do
6:        \( d_{i,k} := d_{i,k} - qd_{j,k} \).
7:     end for
8:   end for
9: end for

In the PSLQ paper [9], size reduction is called Hermite reduction. To avoid confusion with the Hermite Normal Form for integral matrices or the Hermite reduction in the integration of algebraic functions [12] (also for creative telescoping) and to be consistent with the similar process used in lattice reduction algorithms, we replace “Hermite reduction” by “size reduction”.

**Algorithm 2** (BergmanSwap)

**Input:** A lower trapezoidal \( n \times (n-1) \) matrix \( H = (h_{i,j}) \) with \( h_{i,j} = 0 \) if \( j > i \) and \( h_{j,j} \neq 0 \), and a parameter \( \gamma > 2/\sqrt{3} \).

**Output:** A unimodular matrix \( D \) resulting from exchange two rows of the identity matrix.

1: \( D := I_n \).
2: Choose \( r \) such that \( \gamma r |h_{r,r}| = \max_{j \in \{1, \ldots, n-1\}} \{ \gamma j \cdot |h_{j,j}| \} \), and then swap the \( r \)-th row and the \((r + 1)\)-th row of \( D \).

After a Bergman swap of \( H \), \( DH \) usually is not lower trapezoid. We may multiply an orthogonal matrix \( Q \) from right such that \( HQ \) is a lower trapezoid matrix again. This procedure is called Corner, which is equivalent to perform LQ-decomposition on \( H \) (QR-decomposition on \( H^T \)). Suppose after a Bergman swap, the \( r \)-th and \((r + 1)\)-th rows of \( H \) are swapped. Let

\[
\eta = h_{r,r}, \quad \beta = h_{r+1,r}, \quad \lambda = h_{r+1,r+1}, \quad \delta = \sqrt{\beta^2 + \lambda^2}.
\]

Then we can give the following explicit formula for Corner instead of LQ-decomposition.
Algorithm 3 (Corner)

**Input:** A $n \times (n - 1)$ matrix $H$ that is obtained by a Bergman swap with the $r$-th and $(r + 1)$-th rows swapped, where $r < n - 1$.

**Output:** An orthogonal matrix $Q$ such that $HQ$ is the L-factor of the LQ-decomposition on $H$.

1: Return $Q = (q_{i,j}) \in \mathbb{R}^{(n-1)\times(n-1)}$ with

$$q_{i,j} = \begin{cases} \beta/\delta & \text{if } i = r, j = r, \\ -\lambda/\delta & \text{if } i = r, j = r + 1, \\ \lambda/\delta & \text{if } i = r + 1, j = r, \\ \beta/\delta & \text{if } i = r + 1, j = r + 1, \\ 1 & i = j \neq r \text{ or } i = j \neq r + 1, \\ 0 & \text{otherwise.} \end{cases}$$

Now, we are ready to give the following description of the PSLQ algorithm. Note that we suppose that $\alpha \in \mathbb{R}^n$ has integer relations. In fact, this hypothesis is reasonable, because Babai, Just and Meyer auf der Heide [1] showed that it is not possible to decide whether there exists a relation for given input $\alpha \in \mathbb{R}^n$. In addition, we omit an early termination condition that checks whether there exists a column of $B$ that is an integer relation, because it does not impact the analysis of the worst case.

Algorithm 4 (PSLQ)

**Input:** A $n$-dimensional vector $\alpha = (\alpha_1, \cdots, \alpha_n)$ with $\|\alpha\| = 1$ (suppose that $\alpha$ has integer relations) and $\gamma > 2/\sqrt{3}$.

**Output:** An integer relation $m$ for $\alpha$.

1: Construct $H_\alpha$ as in formula (2.1). Set $H := H_\alpha$. Set the $n \times n$ matrices $A$ and $B$ to the identity matrix $I_n$.

2: Let $D := \text{SizeReduce}(H)$. Update $\alpha := \alpha D^{-1}, H := DH, A := DA$, and $B := BD^{-1}$.

3: if $h_{n,n-1} = 0$ then
4: Return the $(n-1)$-th column of $B$.
5: end if

6: Let $D := \text{BergmanSwap}(H, \gamma)$. (Suppose the swap positions are $r$ and $r + 1$.)
7: Update $\alpha := \alpha D^{-1}, H := DH, A := DA$, and $B := BD^{-1}$.
8: if $r < n - 1$ then
9: Let $Q = \text{Corner}(H)$ and update $H := HQ$.
10: end if
11: Goto step 2.

Remark 2.2. At the beginning, the hyperplane matrix $H_\alpha$ has all diagonal elements nonzero. During the algorithm, all diagonal elements of $H$ keep always to be nonzero till the termination of PSLQ.

Theorem 2.3 ([9, Theorem 2]). Assume that $\alpha \in \mathbb{R}^n$ has integer relations. Let $\lambda_\alpha$ be the least $2$-norm of relations for $\alpha$. Then PSLQ will find an integer relation
for $\alpha$ in no more than

$$\left( \frac{n}{2} \right) \log \left( \frac{n-1}{\lambda_0} \right) \log \tau$$

Bergman swaps, where $\tau = \frac{1}{\sqrt{1/4 + 1/\gamma^2}}$ with $\gamma > 2/\sqrt{3}$.

3. The PSLQ Algorithm

The termination of PSLQ requires to check whether $h_{n,n-1} = 0$. When input data $\alpha$ with integer relation are exact, it will hold that $h_{n,n-1} = 0$ after finitely many Bergman swaps. And hence the output is an integer relation of $\alpha$. However, when input data is an approximation of $\alpha$, there may not exist an integer relation of $\alpha$. So $h_{n,n-1}$ usually is not equal to zero. This leads to non-termination of PSLQ. Therefore, we need to explore the termination condition of PSLQ for empirical data.

3.1. An Invariant Relation for PSLQ. Indeed, the quantity $h_{n,n-1}$ plays a very important role in PSLQ, not only for exact data, but also for empirical data. The following theorem gives a relationship between the $(n - 1)$-column of $B$ ($= A^{-1}$) in PSLQ and $h_{n,n-1}$, which will be shown to be crucial for the study of termination of PSLQ with empirical data.

Denote by $H(k)$ the matrix $H$ after exactly $k$ Bergman swaps of PSLQ.

**Theorem 3.1.** Assume that $H(k) = AH_{\alpha}Q$, where $H(k) = (h_{i,j}(k))$ is a lower trapezoidal matrix. Set $(z_1(k), \cdots, z_{n-1}(k), z_n(k)) = (\alpha_1, \cdots, \alpha_{n-1}, \alpha_n)A^{-1}$. Then, it holds that

$$|z_{n-1}(k)| \leq \sqrt{\alpha_{n-1}^2 + \alpha_n^2|h_{n,n-1}(k)|}.$$

**Proof.** From

$$(z_1(k), \cdots, z_{n-1}(k), z_n(k))H(k) = \alpha A^{-1}AH_{\alpha}Q = \alpha H_{\alpha}Q = 0$$

it follows that

$$z_{n-1}(k)h_{n-1,n-1}(k) + z_n(k)h_{n,n-1}(k) = 0.$$

If $h_{n-1,n-1}(k) = 0$ then the last column of $A^{-1}$ is an integer relation for $\alpha$. Now we assume that $h_{n-1,n-1}(k) \neq 0$. Then, it is obtained that

$$z_{n-1}(k) = -\frac{z_n(k)}{h_{n-1,n-1}(k)}h_{n,n-1}(k). \quad (3.1)$$

We claim that $\left| \frac{z_n(k)}{h_{n-1,n-1}(k)} \right|$ does not increase as $k$ increases. At step 1 of Algorithm 4, when the size reduction is performed on row $i \leq n - 1$ of $H$, $z_n$ and $h_{n-1,n-1}$ are unchanged, so $h_{n-1,n-1}$ is unchanged. When $i = n$, the size reduction matrix is as follows

$$D = \begin{pmatrix}
1 & 0 & 0 & \cdots & 0 & 0 \\
0 & 1 & 0 & \cdots & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & 0 & \cdots & 1 & 0 \\
k_1 & k_2 & k_3 & \cdots & k_{n-1} & 1
\end{pmatrix} = \begin{pmatrix}
I_{n-1} & 0 \\
K & 1
\end{pmatrix},$$

\[\begin{array}{c}
Bergman swaps, where \tau = 1/\sqrt{1/4 + 1/\gamma^2} with \gamma > 2/\sqrt{3}.
\end{array}\]
where $K = (k_1, \ldots, k_{n-1})$ is an integer vector, and $I_{n-1}$ is the $(n - 1) \times (n - 1)$ identify matrix. Its inverse is

$$D^{-1} = \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 1 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 1 & 0 \\ -k_1 & -k_2 & -k_3 & \cdots & -k_{n-1} & 1 \end{pmatrix} = \begin{pmatrix} I_{n-1} & 0 \\ -K & 1 \end{pmatrix}.$$  

It is easy to see that the $n$-th column of $A^{-1}D^{-1}$ is the same as that of $A^{-1}$. Therefore, $z_n$ is unchanged. On the other hand, $h_{n-1,n-1}$ is also unchanged after size reduction. Hence, $h_{n-1,n-1}$ is unchanged. In step 3 and step 4 of Algorithm 4, the Bergman swap is performed between the $r$-th and $(r + 1)$-th rows. When $r < n - 2$, it is obvious that $z_n$ and $h_{n-1,n-1}$ are unchanged. When $r = n - 2$, the columns $n - 2$ and $n - 1$ of $A^{-1}$ are swapped. So the $n$-th column of $A^{-1}$ is unchanged and $z_n$ is also unchanged, that is $z_n(k+1) = z_n(k)$, while $h_{n-1,n-1}$ is changed as follows. Before step 3, let $\eta = h_{n-2,n-2}(k)$, $\beta = h_{n-1,n-2}(k)$, $\lambda = h_{n-1,n-1}(k)$ and $\delta = \sqrt{\beta^2 + \lambda^2}$. Then we have

$$\begin{pmatrix} \eta \\ \beta \end{pmatrix} \xrightarrow{\text{step 3}} \begin{pmatrix} \beta \\ \eta \end{pmatrix} \xrightarrow{\text{step 4}} \begin{pmatrix} \frac{\delta}{\beta} & 0 \\ -\frac{\eta}{\delta} & \frac{\beta}{\delta} \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix}. $$

Therefore, after step 4, the new $h_{n-1,n-1}(k + 1) = -\frac{\eta \lambda}{\delta}$. Since the swap occurs at rows $n - 2$ and $n - 1$, it holds that $|\eta| > |\gamma|$. Note that $|\beta| < \frac{|\eta|}{2}$ yields

$$\frac{\delta}{\beta} = \frac{1}{\sqrt{\frac{\beta^2}{\eta^2} + \frac{\lambda^2}{\eta^2}}} > \frac{1}{\frac{\beta}{\gamma} + \frac{\lambda}{\gamma}} = \tau. $$

So, it follows that

$$|h_{n-1,n-1}(k + 1)| = \frac{\delta}{\beta} > \tau |\lambda|. $$

Hence, it holds that

$$\frac{z_n(k + 1)}{h_{n-1,n-1}(k + 1)} < \frac{z_n(k)}{\lambda} = \frac{1}{\tau} \left| \frac{z_n(k)}{h_{n-1,n-1}(k)} \right|. $$

Since $\frac{1}{\tau} < 1$, it implies that $\frac{z_n}{h_{n-1,n-1}}$ decreases. When $r = n - 1$, rows $n - 1$ and $n$ of $H$ are swapped, so are columns $n - 1$ and $n$ of $A^{-1}$. Hence $h_{n-1,n-1}$ and $h_{n,n-1}$ are swapped, and $z_{n-1}$ and $z_n$ are exchanged. Therefore, $h_{n-1,n-1}(k + 1) = h_{n-1,n-1}(k)$ and $z_n(k + 1) = z_{n-1}(k)$. From formula (3.1), it follows that

$$z_n(k + 1) = z_{n-1}(k) = -\frac{h_{n,n-1}(k)}{h_{n-1,n-1}(k)} z_n(k) = -\frac{h_{n-1,n-1}(k + 1)}{h_{n-1,n-1}(k)} z_n(k). $$

In this case, $\frac{z_n}{h_{n-1,n-1}}$ remains unchanged. Up to now, we have shown that $\frac{z_n}{h_{n-1,n-1}}$ either decreases or remains unchanged after the $(k + 1)$-th iteration of PSLQ. At the beginning of PSLQ, we have that $z_n(1) = \alpha_n$ and $h_{n-1,n-1}(k) = \frac{\alpha_n}{\sqrt{\alpha_n^2 + \alpha_n^2}}$. Hence

$$\frac{z_n(k)}{h_{n-1,n-1}(k)} \leq \frac{z_n(1)}{h_{n-1,n-1}(1)} \leq \sqrt{\frac{\alpha_n^2}{\alpha_n^2 + \alpha_n^2}}.$$
which completes the proof.

The property presented in Theorem 3.1 is an invariant of PSLQ in the sense that it always holds during the algorithm. Furthermore, Theorem 3.1 can be used to design an algorithm to find approximate integer relations in the following sense. In fact, if we take the \((n-1)\)-th column of \(B\) as an approximate integer relation for \(\alpha\), Theorem 3.1 gives an error estimate, i.e., if PSLQ returns the \((n-1)\)-th column of \(B\), denoted by \(m\), when \(|h_{n,n-1}| < \varepsilon_2\), then

\[
|\langle \alpha, m \rangle| \leq \sqrt{\alpha^2_{n-1} + \alpha^2_n \varepsilon_2}.
\]

Now we present the algorithm as follows.

**Algorithm 5 (PSLQ\(_{\varepsilon}\))**

**Input**: A lower trapezoidal matrix \(H \in \mathbb{R}^{n \times (n-1)}\) with all diagonal entries nonzero, \(\varepsilon_2 > 0\) and \(\gamma > 2/\sqrt{3}\).

**Output**: An \(n\)-dimensional integer vector \(m\).

1: Set the \(n \times n\) matrices \(A\) and \(B\) to the identity matrix \(I_n\).
2: Let \(D := \text{SizeReduce}(H)\). Update \(H := DH\), \(A := DA\), and \(B := BD^{-1}\).
3: Let \(m\) be the \((n-1)\)-th column of \(B\).
4: if \(|h_{n,n-1}| < \varepsilon_2\) then
5: Return \(m\).
6: end if
7: Let \(D := \text{BergmanSwap}(H, \gamma)\). (Suppose the swap positions are \(r\) and \(r + 1\).)
8: Update \(H := DH\), \(A := DA\), and \(B := BD^{-1}\).
9: if \(r < n - 1\) then
10: Let \(Q = \text{Corner}(H)\) and update \(H := HQ\).
11: end if
12: Goto step 2.

Besides the termination condition is replaced by \(|h_{n,n-1}| < \varepsilon_2\), the main difference of PSLQ\(_{\varepsilon}\) from PSLQ is that the input is changed as a more general lower trapezoidal matrix which may not satisfy the fine structure in (2.1). The remainder of this section will be devoted to analyze PSLQ\(_{\varepsilon}\).

### 3.2. Termination and Complexity.

We now show that PSLQ\(_{\varepsilon}\) terminates after finitely many number of Bergman swaps stated in the following theorem.

**Theorem 3.2.** Given \(H \in \mathbb{R}^{n \times (n-1)}\), PSLQ\(_{\varepsilon}\) terminates within

\[
\frac{n(n+1)((n-1)\log \gamma + \log \frac{1}{\varepsilon_2})}{2 \log \tau}
\]

Bergman swaps, where \(\tau = 1/\sqrt{1/4 + 1/\gamma^2}\).

**Proof.** Define the \(\Pi\) function after \(k\) Bergman swaps as follows

\[
\Pi(k) = \prod_{j=1}^{n-1} \max \left( |h_{i,j}(k)|, \frac{h_{\max}(k)}{\gamma^{n-1}} \right)^{n-j},
\]

where \(h_{\max}(k)\) is the maximum of \(|h_{i,j}(k)|\) for \(i = 1, 2, \ldots, n - 1\). Then the proof is similar to the proof of [9, Theorem 2]; see Appendix B. \(\square\)
Note that if $H$ is the hyperplane matrix for an $\alpha \in \mathbb{R}^n$ and $\alpha$ has an integer relation, let $M_\alpha$ be the minimal 2-norm of integer relations for $\alpha$. Then from [9, Theorem 1], it holds that $\frac{1}{\gamma}$ of $M_\alpha$. From inequality (B.2), it is obtained that

$$k \leq \frac{n(n-1)((n-1)\log \gamma + \frac{1}{\gamma} \log \frac{1}{\gamma(n(k_\text{max})^2)})}{2 \log \tau} \leq \frac{n(n-1)((n-1)\log \gamma + \log M_\alpha)}{2 \log \tau},$$

which is the same as [9, Theorem 2].

3.3. Perturbation Analysis of PSLQ. Before we present the technical details, we recall some notations. For the intrinsic data $\alpha$, we assume that we can only obtain the corresponding empirical data $\bar{\alpha}$ with $\|\alpha - \bar{\alpha}\|_2 < \varepsilon_1$. For $\bar{\alpha}$, we can construct its hyperplane matrix $H_{\bar{\alpha}}$ as in Definition 2.1. But we do not use $H_{\bar{\alpha}}$ as the input matrix for PSLQ. Instead, we use $\bar{H}_\alpha$ to represent a more general perturbation to $H_\alpha$, including round-off errors in computing $H_\alpha$, which only keeps the lower trapezoidal structure and satisfies

$$\|\bar{H}_\alpha - H_\alpha\|_F \leq \varepsilon_3,$$

where $\|\cdot\|_F$ is the matrix Frobenius norm. Suppose that one wants to find an integer relation for $\alpha \in \mathbb{R}^n$ by using PSLQ, the input is $\bar{H}_\alpha$, the termination condition is $|h_{n,n-1}| < \varepsilon_2$ and the output is $m$. We investigate the relations among $\|(m, \alpha)\|$, $\varepsilon_2$ and $\varepsilon_3$.

Denote by $H_{[1..n-1]}$ the submatrix of $H_\alpha$ that consists of the first $n-1$ rows and the first $n-1$ columns. It follows from (3.2) that $\|H_{[1..n-1]} - H_{[1..n-1]}\|_F \leq \varepsilon_3$.

First, we give explicit formulae for the F-norm of $H_{[1..n-1]}$ and $H_{[1..n-1]}^{-1}$; see Appendix A for the proof.

Lemma 3.3. Let the notations be as above. Then

$$\|H_{[1..n-1]}^{-1}\|_F^2 = (n-2) + \frac{\|\alpha\|^2}{\alpha_2^2},$$

$$\|H_{[1..n-1]}\|_F^2 = (n-2) + \frac{\alpha_2^2}{\|\alpha\|^2}.$$

The following lemma enables us to give an estimation on $\|H_{[1..n-1]}^{-1}\|_F$.

Lemma 3.4 ([10, Theorem 2.3.4]). Let $A$ be a nonsingular matrix with perturbation $E$. Let $\|\cdot\|$ denote any matrix norm satisfying inequality $\|BC\| \leq \|B\| \|C\|$ for any matrices $B$ and $C$. If $\|EA^{-1}\| < 1$, then $A + E$ is nonsingular, and it holds

$$\|(A + E)^{-1} - A^{-1}\| \leq \frac{\|EA^{-1}\|}{1 - \|EA^{-1}\|} \|A^{-1}\|.$$

Applying the above lemma to $H_{[1..n-1]}$ yields the following corollary.

Corollary 3.5. Let $H_{\bar{\alpha}} = H_\alpha + \Delta H_\alpha$ and $\|\Delta H_\alpha\|_F < \varepsilon_3$, $H_{[1..n-1]}$ and $\bar{H}_{[1..n-1]}$ denote submatrices consisting of the first $(n-1)$ rows and the first $(n-1)$ columns of $H_\alpha$ and $\bar{H}_\alpha$ respectively. When $\varepsilon_3 < \frac{1}{\|H_{[1..n-1]}^{-1}\|_F}$, $\bar{H}_{[1..n-1]}$ is nonsingular and it holds that

$$\|\bar{H}_{[1..n-1]}^{-1}\|_F \leq \frac{1}{1 - \varepsilon_3 \|H_{[1..n-1]}^{-1}\|_F} \|H_{[1..n-1]}^{-1}\|_F.$$
Lemma 3.7. \( \square \)

Consider the linear system \((1)\) then it reduces to the following system:

\[
\| \Delta H_{[1..n-1]} H_{[1..n-1]}^{-1} \|_F \leq \| \Delta H_{[1..n-1]} \|_F \cdot \| H_{[1..n-1]}^{-1} \|_F \\
< \varepsilon_3 \cdot \| H_{[1..n-1]}^{-1} \|_F < 1.
\]

From Lemma 3.4, \( \mathcal{H}_{[1..n-1]} \) is nonsingular and it follows that

\[
\| \mathcal{H}_{[1..n-1]}^{-1} \|_F < \frac{1}{1 - \| \Delta H_{[1..n-1]} H_{[1..n-1]}^{-1} \|_F \cdot \| H_{[1..n-1]}^{-1} \|_F}.
\]

This completes the proof. \( \square \)

Corollary 3.5 shows that when \( \varepsilon_3 < 1/\| H_{[1..n-1]}^{-1} \|_F \), it holds that \( \mathcal{H}_{i,i} \neq 0 \) for \( i = 1, \ldots, n-1 \). Denote by \( \mathbf{\bar{\alpha}} = (\mathbf{\bar{\alpha}}_1, \ldots, \mathbf{\bar{\alpha}}_n) \) a unit real vector satisfying \( \mathbf{\bar{\alpha}} \mathbf{H}_n \mathbf{\alpha} = 0 \). Without loss of generality, we assume that \( \mathbf{\bar{\alpha}_n} \neq 0 \). Otherwise we can deduce \( \mathbf{\bar{\alpha}} = 0 \), which contradicts to that \( \mathbf{\bar{\alpha}} \) is a unit vector. (In fact, since \( \alpha_n \mathbf{\bar{h}}_{n-1,n-1} + \mathbf{\bar{a}_n} \mathbf{\bar{h}}_{n,n-1} = 0 \) and \( \mathbf{\bar{h}}_{n-1,n-1} \neq 0 \) we have \( \mathbf{\bar{\alpha}_n} = 0 \) implies \( \mathbf{\bar{a}_n} = 0 \). Similarly, \( \mathbf{\bar{a}_i} = 0 \) for \( i = 1, 2, \ldots, n-2 \).) Moreover, we can choose vector \( \mathbf{\bar{\alpha}} \) with \( \mathbf{\bar{\alpha}_n} > 0 \). Next, we give a nonzero lower bound on \( \mathbf{\bar{\alpha}_n} \).

Lemma 3.6. Let \( \mathbf{\xi} = (\xi_1, \cdots, \xi_{n-1}, 1) \) be a real vector with \( \| \mathbf{\xi} \| \leq M \), and assume \( \mathbf{\beta} = (\beta_1, \cdots, \beta_{n-1}, \beta_n) = \| \mathbf{\xi} / \| \mathbf{\xi} \| \) to be a unit vector. Then it holds that \( |\beta_n| \geq \frac{1}{M} \).

Proof. According to assumptions,

\[
1 = \| \mathbf{\beta} \| = \| \beta_n \left( \frac{\beta_1}{\beta_n}, \cdots, \frac{\beta_{n-1}}{\beta_n}, 1 \right) \| = \| \beta_n \mathbf{\xi} \| \leq |\beta_n| \cdot \| \mathbf{\xi} \| \leq |\beta_n|M.
\]

The proof of lemma is finished. \( \square \)

The above lemma enables us to give a lower bound of some component of a unit vector.

Lemma 3.7. Let \( \mathbf{\bar{\alpha}} = (\mathbf{\bar{\alpha}}_1, \cdots, \mathbf{\bar{\alpha}}_{n-1}, \mathbf{\bar{\alpha}}_n) \) be a unit vector such that \( \mathbf{\bar{\alpha}} \mathbf{H}_n \mathbf{\alpha} = 0 \). If \( \varepsilon_3 \) given in (3.2) is less than \( \frac{\alpha_n}{\sqrt{(n-2)\alpha_n^2 + 1}} \), then

\[
|\mathbf{\bar{\alpha}_n}| \geq \frac{\alpha_n}{2\sqrt{1 - \alpha_n^2} \sqrt{(n-2)\alpha_n^2 + 1} + 2\alpha_n}.
\]

Proof. Consider the linear system \((x_1, \cdots, x_n) \mathbf{H}_n = 0 \) with \( x_i \) unknowns for \( i = 1, 2, \cdots, n \). Since the rank of \( \mathbf{H}_n \) is at most \( n-1 \), we can assume that \( x_n = 1 \), then it reduces to the following system:

\[
(x_1, \cdots, x_{n-1}, 1) \mathbf{H}_{[1..n-1]} = -(\mathbf{\bar{h}}_{n,1}, \cdots, \mathbf{\bar{h}}_{n,n-1}).
\]
If $\varepsilon_3 < \frac{\alpha_n}{2\sqrt{(n-2)\alpha_n^2 + 1}}$, then $\overline{H}_{[1..n-1]}$ is nonsingular by Lemma 3.3 and Corollary 3.5, so $(x_1, \cdots, x_{n-1}) = -\overline{(h_{n,1}, \cdots, h_{n,n-1})}\overline{H}_{[1..n-1]}^{-1}$. Hence, it holds that

$$
\|(x_1, \cdots, x_{n-1})\|_2 \leq \|(\overline{h}_{n,1}, \cdots, \overline{h}_{n,n-1})\|_2 \|\overline{H}_{[1..n-1]}^{-1}\|_2 \\
\leq \|(\overline{h}_{n,1}, \cdots, \overline{h}_{n,n-1})\|_2 \|\overline{H}_{[1..n-1]}^{-1}\|_F \\
\leq \left(\frac{1 - \alpha_n^2 + \alpha_n}{2\sqrt{(n-2)\alpha_n^2 + 1}}\right)^2 \|\overline{H}_{[1..n-1]}^{-1}\|_F \\
= 2\sqrt{1 - \alpha_n^2 \sqrt{(n-2)\alpha_n^2 + 1}} + 1 \\
= \frac{2\sqrt{1 - \alpha_n^2 \sqrt{(n-2)\alpha_n^2 + 1} + 1 + 2\alpha_n}}{\alpha_n}.
$$

Thus, it is obtained that

$$
\|(x_1, \cdots, x_{n-1}, x_n)\|_2 \leq \|(x_1, \cdots, x_{n-1})\|_2 + 1 \\
= 2\sqrt{1 - \alpha_n^2 \sqrt{(n-2)\alpha_n^2 + 1} + 1} + 1 + 2\alpha_n.
$$

From Lemma 3.6, it follows that

$$
|\overline{a}_n| \geq \frac{1}{\|x_1, x_2, \cdots, x_{n}\|} \geq \frac{\alpha_n}{2\sqrt{1 - \alpha_n^2 \sqrt{(n-2)\alpha_n^2 + 1} + 1 + 2\alpha_n}}.
$$

The proof of the lemma is finished. \(\square\)

We now give a main theorem of this paper, which can be seen as a forward error analysis of PSLQ, for the perturbation introduced in (3.2).

**Theorem 3.8.** Given a real vector $\alpha = (\alpha_1, \cdots, \alpha_n)$, let $H_\alpha$ be the hyperplane matrix constructed as in (2.1). Let $\overline{H}_\alpha$ be an approximate matrix of $H_\alpha$ with $\|H_\alpha - \overline{H}_\alpha\|_F < \varepsilon_3 < \frac{\alpha_n}{2\sqrt{(n-2)\alpha_n^2 + 1}}$. Let $A$ be the unimodular matrix and $Q$ the orthogonal matrix such that $H = (h_{i,j}) = \overline{A}\overline{H}_\alpha Q$ is a lower trapezoidal matrix at the termination of PSLQ, with $|h_{n,n-1}| < \varepsilon_2$. Let $m$ denote the $(n-1)$-th column of $A^{-1}$. Then

$$
\|\langle \alpha, m \rangle \| < C \cdot (\|m\|\varepsilon_3 + \alpha_n\varepsilon_2),
$$

where $C = \frac{2\sqrt{(n-2)\alpha_n^2 + 1 + \alpha_n}}{\alpha_n}.

**Proof.** Suppose that PSLQ returns $m$ with $\overline{H}_\alpha$ as the hyperplane matrix, when $|h_{n,n-1}| < \varepsilon_2$. Then this process can be seen as running PSLQ, for a unit vector $\overline{\mathbf{a}}$ satisfying $\overline{\mathbf{a}}\overline{H}_\alpha = 0$. According to Theorem 3.1, we have $|\langle \overline{\mathbf{a}}, m \rangle | \leq \varepsilon_2$. Now we consider the following system

$$
\overline{H}_\alpha \mathbf{c} = \mathbf{m} + (0,0,\cdots,0,b)^T
$$

where $\mathbf{c} = (c_1, c_2, \cdots, c_{n-1})^T$ is the unknown vector. We have that

$$
0 = \overline{\mathbf{a}}\overline{H}_\alpha \mathbf{c} = \langle \overline{\mathbf{a}}, \mathbf{m} \rangle + \overline{\mathbf{a}}_n b.
$$
Hence $\overline{\alpha}_n b = -\langle \overline{\alpha}, m \rangle$, and we have
\[ |b| < \frac{\epsilon_2}{\overline{\alpha}_n}. \]

Meanwhile, it implies
\[ |\langle \alpha, m \rangle| = |\alpha \overline{H}_\alpha c - \alpha_n b| \leq |\alpha \overline{H}_\alpha c| + |\alpha_n||b| \]
\[ \leq |\alpha(\overline{H}_\alpha - H_\alpha)c| + |\alpha_n||b| \]
\[ \leq \|\alpha\|\|\overline{H}_\alpha - H_\alpha\|_2 \|c\| + |\alpha_n||b| \]
\[ \leq \|\alpha\| \|c\| \epsilon_3 + |\alpha_n| \epsilon_2. \]

Since $\epsilon_3 < \frac{\alpha_n}{2\sqrt{(n-2)\alpha_n^2+1}}$, by Lemma 3.7, it follows that
\[ (3.4) \quad |\langle \alpha, m \rangle| < \|\alpha\| \|c\| \epsilon_3 + 2(\sqrt{1 - \frac{\alpha_n^2}{(n-2)\alpha_n^2+1}} + \alpha_n)\epsilon_2. \]

The first $n - 1$ equations of (3.3) give a square system
\[ \overline{H}_{[1..n-1]} \begin{pmatrix} c_1 \\ \vdots \\ c_{n-1} \end{pmatrix} = \begin{pmatrix} m_1 \\ \vdots \\ m_{n-1} \end{pmatrix}. \]

Then it is obtained that
\[ \|c\| \leq \overline{H}_{[1..n-1]}^{-1} \left\| \begin{pmatrix} m_1 \\ \vdots \\ m_{n-1} \end{pmatrix} \right\| \leq \overline{H}_{[1..n-1]}^{-1} \|F\| \|m\|. \]

Since $\epsilon_3 < \frac{\alpha_n}{2\sqrt{(n-2)\alpha_n^2+1}}$, by Corollary 3.5 we have
\[ \|c\| \leq \frac{1}{1 - \epsilon_3 \|\overline{H}_{[1..n-1]}^{-1}\|_F} \|\overline{H}_{[1..n-1]}^{-1}\|_F \|m\|_2 \]
\[ < 2 \|\overline{H}_{[1..n-1]}^{-1}\|_F \|m\|_2 < \frac{2\sqrt{(n-2)\alpha_n^2+1}}{\alpha_n} \|m\|_2. \]

Substituting the above inequality into (3.4) yields
\[ |\langle \alpha, m \rangle| < \|\alpha\| \|c\| \epsilon_3 + 2(\sqrt{1 - \frac{\alpha_n^2}{(n-2)\alpha_n^2+1}} + \alpha_n)\epsilon_2 \]
\[ < \frac{2\sqrt{(n-2)\alpha_n^2+1}}{\alpha_n} \|m\| \epsilon_3 + 2(\sqrt{1 - \frac{\alpha_n^2}{(n-2)\alpha_n^2+1}} + \alpha_n)\epsilon_2 \]
\[ < \frac{2(\sqrt{(n-2)\alpha_n^2+1}}{\alpha_n} \|m\| \epsilon_3 + 2(\sqrt{1 - \frac{\alpha_n^2}{(n-2)\alpha_n^2+1}} + \alpha_n)\epsilon_2 \]
\[ = \frac{2(\sqrt{(n-2)\alpha_n^2+1}}{\alpha_n} (\|m\| \epsilon_3 + \alpha_n\epsilon_2). \]

The theorem is proved. \( \Box \)

Although the quantity $|\langle \alpha, m \rangle|$ usually is nonzero for empirical data, it somewhat measures how close $m$ is to a true integer relation for $\alpha$. So it can be seen as output error. In this sense, Theorem 3.8 says that if a perturbation of the input $H_\alpha$ is small enough then the “output error” of PSLQ can be also small. Roughly speaking,
if we fix the termination condition \( \varepsilon_2 \) to be a tiny number, then the “output error” is amplified by a factor \( C \cdot \| m \| \) at most.

4. PSLQ\(_r\) with Empirical Data

Aiming to obtain \( m \) by PSLQ\(_r\), such that \( |\langle \alpha, m \rangle| < \epsilon \), we study how to determine the error control parameters \( \varepsilon_1, \varepsilon_2 \) and \( \varepsilon_3 \) in this section.

4.1. Error Control of PSLQ\(_r\)

Lemma 4.1. Let \( \alpha = (\alpha_1, \cdots, \alpha_n) \) be an \( n \)-dimensional unit vector with \( |\alpha_n| = \max_i |\alpha_i| \) and let \( \bar{\alpha} \) be its approximation. Construct \( H_{\alpha} \) and \( H_{\bar{\alpha}} \) as in (2.1) for \( \alpha \) and \( \bar{\alpha} \) respectively. If \( \| \alpha - \bar{\alpha} \| < \frac{1}{8n} \), then it holds that

\[
\| H_{\alpha} - H_{\bar{\alpha}} \| F < n^2 \| \alpha - \bar{\alpha} \|. 
\]

Proof. Let \( s_i = \frac{\sqrt{\sum_{k=1}^{n} \alpha_k^2}}{s_i} \), \( \bar{s}_i = \frac{\sqrt{\sum_{k=1}^{n} \alpha_k^2}}{s_i} \), \( b_i = (0, \cdots, 0, \alpha_i, \cdots, \alpha_n) \) and \( \bar{b}_i = (0, \cdots, 0, \bar{\alpha}_i, \cdots, \bar{\alpha}_n) \). It obviously holds that \( \| b_i - \bar{b}_i \| \leq \| \alpha - \bar{\alpha} \| \). So, it is obtained that \( |s_i - \bar{s}_i| = \| b_i \| - \| \bar{b}_i \| \leq \| \alpha - \bar{\alpha} \| \). By the way, from \( |\alpha_n| = \max_i |\alpha_i| \) and \( |\bar{\alpha}| = 1 \), it follows that \( |\alpha_n| \geq \frac{1}{\sqrt{n}} \). If \( \| \alpha - \bar{\alpha} \| < \frac{1}{8n} \), then it holds that \( |\alpha_n| > \frac{1}{2\sqrt{n}} \).

Recall \( H_{\alpha} = (h_{i,j}) \) and

\[
h_{i,j} = \begin{cases} \frac{s_i s_j + 1}{s_i s_j} & \text{if } i = j \\ \frac{s_i s_j}{s_i s_j + 1} & \text{else if } i > j \\ 0 & \text{otherwise.} \end{cases}
\]

Let us consider the error of \( \frac{s_i s_j + 1}{s_i s_j} \):

\[
\left| \frac{s_i s_j + 1}{s_i s_j} - \frac{s_i s_j + 1}{s_i s_j} \right| = \left| \frac{s_i s_j + 1}{s_i s_j} - \frac{s_i s_j + 1}{s_i s_j} \right| = \frac{|s_i s_j + 1|}{s_i s_j} \leq s_i s_j + 1 \\
\leq \frac{2}{s_i} \| \alpha - \bar{\alpha} \| \leq \frac{2}{s_i} \| \alpha - \bar{\alpha} \| \leq 4\sqrt{n} \| \alpha - \bar{\alpha} \|
\]

And then consider the error of \( \frac{\alpha_i \alpha_j}{s_j s_j + 1} (i > j) \):

\[
\left| \frac{\alpha_i \alpha_j}{s_j s_j + 1} \right| = \left| \frac{\alpha_i \alpha_j}{s_j s_j + 1} \right| = \left| \frac{\alpha_i \alpha_j}{s_j s_j + 1} \right| = \left| \frac{\alpha_i \alpha_j}{s_j s_j + 1} \right| \\
\leq \frac{1}{s_j s_j + 1} \left( |\alpha_i \alpha_j s_j s_j| + |\alpha_i \alpha_j s_j s_j| + |\alpha_i \alpha_j s_j s_j| + |\alpha_i \alpha_j s_j s_j| \right) \\
\leq \frac{1}{s_j s_j + 1} \left( |\alpha_i \alpha_j s_j s_j| + |\alpha_i \alpha_j s_j s_j| + |\alpha_i \alpha_j s_j s_j| + |\alpha_i \alpha_j s_j s_j| \right)
\]

(4.1)
We need to estimate $\frac{|\alpha_j|}{s_j}$. First, if $|\alpha_j| \leq |\bar{\alpha}_j|$, then it holds that $|\alpha_j| |s_j| \leq 1$. When $|\alpha_j| > |\bar{\alpha}_j|$, it follows that

$$s_j^2 = \bar{\alpha}_j^2 + \cdots + \bar{\alpha}_n^2 = \alpha_j^2 + 2\Delta \alpha_j \alpha_j + \Delta \alpha_j^2 + \bar{\alpha}_{j+1}^2 + \cdots + \bar{\alpha}_n^2,$$

so we have

$$s_j^2 - \alpha_j^2 \geq \sum_{k=j+1}^{n} \bar{\alpha}_k^2 - 2|\Delta \alpha_j||\alpha_j| \geq \bar{\alpha}_n^2 - 2|\Delta \alpha_j|.$$

Note that $|\bar{\alpha}_n| > \frac{1}{2\sqrt{n}}$ and $|\Delta \alpha_j| < \frac{1}{8n}$ when $\|\alpha - \bar{\alpha}\| < \frac{1}{8n}$, which indicate $s_j^2 - \alpha_j^2 \geq \bar{\alpha}_n^2 - 2|\Delta \alpha_j| > \frac{1}{8n} - \frac{1}{8n} = 0$. So it is proved that

$$(4.2) \quad \frac{|\alpha_j|}{s_j} \leq 1$$

when $\|\alpha - \bar{\alpha}\| < \frac{1}{8n}$. Applying (4.2) to (4.1) gives

$$\left| \frac{\alpha_i \alpha_j}{s_j s_{j+1}} - \frac{\bar{\alpha}_i \bar{\alpha}_j}{s_j s_{j+1}} \right| \leq \frac{|s_j - s_j|}{s_j s_{j+1}} + \frac{|s_j - s_{j+1}|}{s_{j+1}} + \frac{|s_j|}{s_j} \left| \frac{|s_j - s_{j+1}|}{s_{j+1}} + \frac{|s_j|}{s_j} \right| \leq \frac{4}{2\sqrt{n}} \|\alpha - \bar{\alpha}\| = 8\sqrt{n}\|\alpha - \bar{\alpha}\|.$$

Under assumption of $\|\alpha - \bar{\alpha}\| < \frac{1}{8n}$, it follows that

$$\|H_\alpha - H_{\bar{\alpha}}\|_F \leq 8\sqrt{n}\sqrt{\frac{n(n-1)}{2} + (n-1)} \|\alpha - \bar{\alpha}\| \leq 8n^{3/2}\|\alpha - \bar{\alpha}\|.$$

The proof is finished. \qed

Now we construct the input $H_\alpha$ of PSLQ$_e$ from empirical data $\bar{\alpha}$. In this paper, we restrict ourselves under exact arithmetic. Particularly, we take $H_{\bar{\alpha}} = H_{\bar{\alpha}}$. Applying this to Theorem 3.8 yields the following particular error control strategy.

**Theorem 4.2.** Let $\alpha \in \mathbb{R}^n$ be a unit vector with $|\alpha_n| = \max_i \{|\alpha_i|\}$ and $\epsilon > 0$. Suppose $\alpha$ has an integer relation with 2-norm bounded from above by $M$. Given empirical data $\bar{\alpha}$ with

$$\|\alpha - \bar{\alpha}\| < \epsilon_1 < \frac{\epsilon}{16MCn^{3/2}},$$

if PSLQ$_e$ with

$$\epsilon_2 < \frac{\epsilon}{2C\alpha_n}$$

returns $m$ with $\|m\| < M$, then $|\langle \alpha, m \rangle| < \epsilon$, where $C = \frac{2(\sqrt{n-2}n^2 + 1 + \alpha_n)}{\alpha_n}$ and $M > 0$.

**Proof.** From Lemma 4.1, it holds that

$$\|H_\alpha - H_{\bar{\alpha}}\|_F = \|H_\alpha - H_{\bar{\alpha}}\|_F < \frac{\epsilon}{2M \cdot C}.$$ Then Theorem 3.8 implies

$$|\langle \alpha, m \rangle| < C \left( \frac{\epsilon}{2M \cdot C} + \alpha_n \epsilon_2 \right) < \frac{\epsilon}{2} + \frac{\epsilon}{2} = \epsilon.$$ The theorem is proved. \qed
4.2. Some Remarks. It is not difficult to verify that Theorem 4.2 still holds for
\( \varepsilon_1 < \frac{\omega}{2MCn^{\frac{1}{2}}} \) and \( \varepsilon_2 < \frac{(1-\omega)\varepsilon_{\alpha}}{\varepsilon_{\alpha}} \), where \( 0 < \omega < 1 \). The error control strategy given in Theorem 4.2 takes \( \omega = 1/2 \). Examples in next section show the effectiveness of this strategy, but, the optimal choice for \( \omega \) is beyond the scope of this paper.

Figure 1 shows the relationships among the main notations of this paper. In this figure, the solid lines indicate the routine of \( \text{PSLQ}_\varepsilon \) for empirical input data \( \bar{\alpha} \) with \( \|\alpha - \bar{\alpha}\| < \varepsilon_1 \). According to Theorem 4.2, if the returned \( m \) by \( \text{PSLQ}_\varepsilon \) satisfies \( \|m\| < M \) then we can guarantee that \( |\langle m, \alpha \rangle| < \varepsilon \).

As mentioned previously, high precision arithmetic must be used for almost all applications of \( \text{PSLQ} \). In practice, Bailey (see, e.g., [2]) suggested that if one wishes to recover a relation for an \( n \)-dimensional vector, with coefficients of maximum size \( \log_{10} G \) decimal digits, then the input vector \( \alpha \) must be specified to at least \( n \log_{10} G \) digits, and one must employ floating-point arithmetic accurate to at least \( n \log_{10} G \) digits. However, there seems no theoretical results about how to decide the precision generally. Theorem 3.8 and 4.2 in this paper can be seen as theoretical sufficient conditions for \( \text{PSLQ} \) with empirical input data. We show in next subsection that these theoretical results indeed give some effective strategies for the input data precision and the termination condition in practice.

4.3. Numerical Examples. In this subsection, we give some examples to illustrate our strategy of error control based on Theorem 4.2. We use our own Maple implementation of \( \text{PSLQ}_\varepsilon \) which takes the running precision \( \text{Digits} \), a target accuracy \( \varepsilon \) and an upper bound on the coefficients of the expected relation \( G \) as its input. (In the procedure, we use \( M = \sqrt{\pi G} \) as its 2-norm bound.) Throughout the following examples, we fix \( \text{Digits} := 200 \) so that it is sufficient to guarantee the correctness and that it can mimic the exact real arithmetic.

**Example 4.3** (Transcendental numbers). Equation (69) of [3] states that \( \beta = (t, 1, \ln 2, \ln^2 2, \pi^2) \in \mathbb{R}^5 \) has an integer relation \( m = (1, -5, 4, -16, 1) \), where

\[
t = \int_0^1 \int_0^1 \left( \frac{x-1}{x+1} \right)^2 \left( \frac{y-1}{y+1} \right)^2 \left( \frac{xy-1}{xy+1} \right)^2 \, dx \, dy.
\]

We try to recover this relation for \( \alpha = \beta/\|\beta\| \).

Because of involving transcendental numbers, we can only obtain empirical data of \( \alpha \). Suppose that the maximum of the coefficients is bounded by \( G = 16 \) and that the gap bound for this example is \( 10^{-6} \). (In fact, by exhaustive search, we can obtain a gap bound that is about \( 6.37 \times 10^{-6} \).) Thus, the target precision \( \varepsilon \) is set as \( \varepsilon = 10^{-5} \). It means that we want to find an integer vector \( m \) such that \( |\langle \alpha, m \rangle| < \varepsilon = 10^{-5} \). According to Theorem 4.2, we obtain that \( \varepsilon_1 \approx 2.60 \times 10^{-11} \).
and \( \epsilon_2 \approx 8.39 \times 10^{-8} \). We run this example in the computer algebra system Maple. After 30 Bergman swaps, the procedure returns a relation \( m = (1, -5, 4, -16, 1) \), which is an exact integer relation for \( \alpha \).

If we do not know a gap bound on \(|\langle m, \alpha \rangle|\), we can test \( \epsilon = 10^{-i} \) for \( i = 1, 2, \ldots, 10 \), where the corresponding \( \epsilon_1 \) and \( \epsilon_2 \) are decided according to Theorem 4.2. As shown in Figure 2, for \( i = 1, 2, 3, 4 \), no correct answer is obtained, but for \( 5 \leq i \leq 10 \) the procedure always returns the same relation \( m \). Further, the difference between \( \lceil -\log_{10} \epsilon_1 \rceil \) and \( \lceil -\log_{10} \epsilon_2 \rceil \) does not change for different \( \epsilon \).

Bailey’s estimation is \( \lceil n \log_{10} G \rceil = 7 \) decimal digits that indicates \( \epsilon_1 < 10^{-7} \), which is relatively compact for the above setting. However, Bailey’s estimation still has the following drawbacks. For one thing, Bailey’s estimation does not suggest when the algorithm terminates, i.e., how to choose \( \epsilon_2 \), while Theorem 4.2 suggests the quantity that \( \epsilon_2 \) should be larger than \( \epsilon_1 \). This is consistent with intuition: the error would be amplified by exact computation with empirical data as input. In fact, if we do not have the error control strategy as indicated by Theorem 4.2, we can only use a trial-and-error approach to decide the termination precision \( \epsilon_2 \), since the procedure may miss the correct answer for an incorrect \( \epsilon_2 \), even with relatively high precision.

For another thing, if we do not know a so tight bound on the maximum coefficient of the relation, instead, for example, we only know \( G \leq 10^5 \). For the same \( \epsilon \), we now have \( \epsilon_1 \approx 4.16 \times 10^{-15} \) and \( \epsilon_2 \approx 8.39 \times 10^{-8} \), for which our procedure work correctly, while at least \( \lceil n \log_{10} G \rceil = 25 \) decimal digits is needed according to Bailey’s estimation, which implies \( \epsilon_1 < 10^{-25} \). For this example, by Bailey’s estimation, \( \lceil -\log_{10} \epsilon_1 \rceil \) increases linearly with \( \lceil \log_{10} G \rceil \), whose slope is \( n = 5 \). According to Theorem 4.2, \( \lceil -\log_{10} \epsilon_1 \rceil \) also increases linearly with \( \lceil \log_{10} G \rceil \), but the slope is about 1 only. In fact, according to Theorem 4.2, we have \( \lceil -\log_{10} \epsilon_1 \rceil \geq \lceil \log G + \log_{10}(16n^{5/2}C) - \log_{10} \epsilon \rceil \).

**Figure 2.** Error control strategy for Example 4.3
Example 4.4 (Algebraic numbers). Let $\alpha = \left(\sqrt[3]{3} + \sqrt[2]{2}\right)^{-1}$ and let $\alpha$ be the normalized vector of $(\alpha^{20}, \alpha^{19}, \cdots, \alpha, 1)$. In this example, we try to recover the coefficients of the minimal polynomial of $\alpha$. Suppose that we know in advance that the $\infty$-norm of the integer relation is at most $G = 7440$.

Bailey’s estimation suggests that $\alpha$ should be computed with $\lceil n \log_{10} G \rceil = 82$ exact decimal digits at least, which implies $\varepsilon_1 < 10^{-82}$. However, PSLQ does not return an relation with coefficient bounded by 7440. This may caused by that Bailey’s estimation is not sufficient to compute an integer relation.

Let us set $\varepsilon = 10^{-89}$ so that $\varepsilon_1 \approx 1.73 \times 10^{-98}$ and $\varepsilon_2 \approx 4.99 \times 10^{-91}$, and our procedure returns an relation

$$m = (49, -1080, 3960, -3360, 80, -108, -6120, -7440, -80, 0, 54, -1560, 40, 0, 0, -12, -10, 0, 0, 0, 1)$$

after 3525 Bergman swaps. It can be checked that this relation exactly corresponds to the coefficients of the minimal polynomial of $\alpha$.

For the same $\varepsilon$ and $\varepsilon_1$, if we do not set $\varepsilon_2$ as suggested by Theorem 4.2, say, $\varepsilon_2 \approx 10^{-96}$, then the procedure misses the correct relation.

If we set $\varepsilon = 10^{-88}$, our procedure does not return the correct answer. This can be seen as an evidence for that the sharp gap bound is near to $10^{-89}$. We also test for $\varepsilon = 10^{-100-i}$ with $i = 1, 2, \cdots, 9$. Each of these tests does not return the correct answer. If we set $\varepsilon$ more strictly, which means paying more precision, for example $\varepsilon = 10^{-100+10i}$ with $i = 1, 2, \cdots, 8$, the procedure always works well and returns the same $m$ as above. The quantities $\lceil -\log_{10} \varepsilon_1 \rceil$ and $\lceil -\log_{10} \varepsilon_2 \rceil$ obtained from Theorem 4.2 are as shown in Figure 3.

From the above two examples, we have the following two observations. Firstly, if one does not decide $\varepsilon_1$ and $\varepsilon_2$ by the error control strategy in Theorem 4.2, then
one may miss the correct relation. Secondly, with an effective $\epsilon$, we always obtain the same relation if we use the error control strategy in Theorem 4.2. In fact, assume that for all arbitrary small $\epsilon > 0$ PSLQ$_\epsilon$ always returns the same relation. Then the relation must be an exact integer relation in the sense that PSLQ$_\epsilon \to m$ for $\epsilon \to 0$. However, assuming without a gap bound, how to decide whether the returned relation is an exact integer relation within finite steps is an open problem.

5. Conclusion

In this paper, we give a new invariant relation of the celebrated integer relation finding algorithm PSLQ, and hence introduce a new termination condition for PSLQ$_\epsilon$. The new termination condition allows us to compute integer relations by PSLQ$_\epsilon$ with empirical data as its input. By a perturbation analysis, we disclose the relationship between the accuracy of the input data ($\epsilon_1$) and the output quality ($\epsilon$, an upper bound on the absolute value of the inner product of the intrinsic data and the computed relation) of the algorithm. Examples show that our error control strategies based on this relationship are very helpful in practice.

We note that all above results presented in this paper are under exact arithmetic computational model. Although we obtain some results about the error control for applications, we did not analyze the algorithm under an inexact arithmetic model, such as floating-point arithmetic. However, we believe that parts of the results in this paper, say Theorem 3.8, would be indispensable in the analysis of a numerical PSLQ algorithm.

In addition, it is an intriguing topic to design and analyze an efficient numerical PSLQ algorithm. For the moment, the main obstacle is to give a reasonable bound on the entries of unimodular matrices produced by the algorithm. Now, we can only give an upper bound that is double exponential with respect to the working dimension, and hence resulting in an exponential time algorithm. Thus, it is a very interesting challenge to obtain an upper bound similar to [16, Lemma 6], in which the upper bound is of single exponential in the dimension.

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APPENDIX A. PROOF OF LEMMA 3.3

We consider the following submatrix of $H_\alpha$, denoted by $H_{[1..n-1]}$:

$$H_{[1..n-1]} = \begin{pmatrix}
\frac{s_1}{s_1} & 0 & 0 & \cdots & 0 & 0 \\
\frac{s_2}{s_2} & \frac{s_3}{s_2} & 0 & \cdots & 0 & 0 \\
\frac{s_3}{s_3} & \frac{s_4}{s_3} & \frac{s_5}{s_3} & \cdots & 0 & 0 \\
\vdots & \vdots & \vdots & \cdots & \vdots & \vdots \\
-\frac{s_{n-1}}{s_{n-1}} & -\frac{s_{n-2}}{s_{n-1}} & -\frac{s_{n-1}}{s_{n-1}} & \cdots & 0 & 0 \\
\frac{s_1}{s_1} & \frac{s_2}{s_2} & \frac{s_3}{s_2} & \frac{s_4}{s_2} & \cdots & \frac{s_n}{s_2}
\end{pmatrix}.$$ 

By linear algebra, its inverse is

$$(A.1) \quad H^{-1}_{[1..n-1]} = \begin{pmatrix}
\frac{s_1}{s_1} & 0 & 0 & \cdots & 0 & 0 \\
\frac{s_2}{s_2} & \frac{s_3}{s_2} & 0 & \cdots & 0 & 0 \\
\frac{s_3}{s_3} & \frac{s_4}{s_3} & \frac{s_5}{s_3} & \cdots & 0 & 0 \\
\vdots & \vdots & \vdots & \cdots & \vdots & \vdots \\
\frac{s_{n-1}}{s_{n-1}} & \frac{s_{n-2}}{s_{n-1}} & \frac{s_{n-1}}{s_{n-1}} & \cdots & 0 & 0 \\
\frac{s_1}{s_1} & \frac{s_2}{s_2} & \frac{s_3}{s_2} & \frac{s_4}{s_2} & \cdots & \frac{s_n}{s_2}
\end{pmatrix}.$$
In the following, we compute the F-norm of $H_{[1..n-1]}^{-1}$. First, consider the $j$-th column of $H_{[1..n-1]}^{-1}$:

$$
\|H_j^{-1}\|^2 = \frac{s_j^2}{s_{j+1}} + \sum_{k=j+1}^{n-1} \frac{\alpha_k^2 \alpha_j^2}{s_k s_{k+1} s_{j+1}} = \frac{s_j^2}{s_{j+1}} + \alpha_j^2 \sum_{k=j+1}^{n-1} \frac{\alpha_k^2}{s_k s_{k+1}}
$$

$$
= \frac{s_j^2}{s_{j+1}} + \alpha_j^2 \sum_{k=j+1}^{n-1} \left( \frac{1}{s_{k+1}} - \frac{1}{s_k} \right) = \frac{s_j^2}{s_{j+1}} + \alpha_j^2 \left( \frac{1}{s_{n}} - \frac{1}{s_{j+1}} \right)
$$

$$
= \frac{s_j^2 - \alpha_j^2}{s_{j+1}} + \frac{s_j^2}{s_{j+1}} = 1 + \frac{\alpha_j^2}{\alpha_n^2}
$$

so we have

$$
\|H_{[1..n-1]}^{-1}\|^2 = \sum_{j=1}^{n-1} \|H_j^{-1}\|^2 = (n-1) + \sum_{j=1}^{n-1} \frac{\alpha_j^2}{\alpha_n^2} = (n-1) + \frac{\|\alpha\|^2 - \alpha_n^2}{\alpha_n^2} = (n-2) + \frac{\|\alpha\|^2}{\alpha_n^2}.
$$

In addition, we can compute the F-norm of $H_{[1..n-1]}$ as follows:

$$
\|H_{[1..n-1]}\|^2 = \|H_{\alpha}\|^2 - \sum_{i=1}^{n-1} \frac{\alpha_i^2 \alpha_i^2}{s_i^2 s_i^2 + 1} = (n-1) - \alpha_n^2 \sum_{i=1}^{n-1} \frac{\alpha_i^2}{s_i^2 s_i^2 + 1}
$$

$$
= (n-1) - \alpha_n^2 \sum_{i=1}^{n-1} \left( \frac{1}{s_i^2} - \frac{1}{s_i^2} \right) = (n-1) - \alpha_n^2 \left( \frac{1}{s_n^2} - \frac{1}{s_1^2} \right)
$$

$$
= (n-1) - 1 + \frac{\alpha_n^2}{\|\alpha\|^2} = (n-2) + \frac{\alpha_n^2}{\|\alpha\|^2},
$$

as claimed in Lemma 3.3.

APPENDIX B. PROOF OF THEOREM 3.2

Define the $\Pi$ function after $k$ Berman swaps as follows

$$
\Pi(k) = \prod_{j=1}^{n-1} \max \left( |h_{i,i}(k)|, \frac{h_{\max}(k)}{\gamma^{n-1}} \right)^{n-j},
$$

where $h_{\max}(k)$ is the maximum of $|h_{i,i}(k)|$ for $i = 1, 2, \ldots, n-1$. It obviously holds that

$$
\Pi(k) = \prod_{j=1}^{n-1} \max \left( |h_{i,i}(k)|, \frac{h_{\max}(k)}{\gamma^{n-1}} \right)^{n-j} \geq \left( \frac{h_{\max}(k)}{\gamma^{n-1}} \right)^{\frac{n(n-1)}{2}}.
$$

First, we assert that $h_{\max}(k) \geq h_{\max}(k+1)$. Size reduction does not affect $h_{i,i}$, neither do $h_{\max}$. Let us consider the change of $h_{\max}$ in the Bergman swap. Let Bergman swap occur at $r$-th row. So we have $|h_{r,r}| \geq \gamma h_{r+1,r+1}$ for $r < n - 1$ and $r = n - 1$. In the case that $r < n - 1$, it is impossible that $h_{\max}(k) = |h_{r+1,r+1}(k)|$ due to $|h_{r,r}| \geq \gamma h_{r+1,r+1}$ with $\gamma > 1$. Hence when $h_{\max}(k) \neq |h_{r,r}(k)|$, Bergman swap does not affect $h_{\max}$. When $h_{\max}(k) = |h_{r,r}(k)|$, after Bergman swap, we have that $h_{r,r}(k + 1) < \frac{1}{\sqrt{h_{r,r}(k)h_{r+1,r+1}(k)}} \leq |h_{r,r}(k)| = h_{\max}(k)$ and $|h_{r+1,r+1}(k + 1)| = \frac{|h_{r,r}(k)h_{r+1,r+1}(k)|}{\sqrt{h_{r,r}(k)h_{r+1,r+1}(k)}} \leq |h_{r,r}(k)| = h_{\max}(k)$. The other $h_{i,i}(k)$ are unchanged. So
it holds $h_{\max}(k) > h_{\max}(k+1)$ for $r < n - 1$. When $r = n - 1$, after Bergman swap, it holds $|h_{n-1,n-1}(k+1)| < \frac{1}{\rho} |h_{n-1,n-1}(k)| < h_{\max}(k)$. Therefore it is obtained that $h_{\max}(k) \geq h_{\max}(k+1)$.

Second, we show that $\Pi(k) > \tau \Pi(k + 1)$. Let Bergman swap occurs at row $r$.

Case $r = n - 1$:

\[
\Pi(k) = \max\{|h_{n-1,n-1}(k)|, \frac{h_{\max}(k)}{\gamma} \} = \frac{|h_{n-1,n-1}(k)|}{\max\{|h_{n-1,n-1}(k+1)|, \frac{h_{\max}(k+1)}{\gamma} \}} = \begin{cases} \frac{|h_{n-1,n-1}(k)|}{\frac{h_{\max}(k+1)}{\gamma}} & \text{when } h_{n-1,n-1}(k) > \frac{h_{\max}(k+1)}{\gamma} \\ \frac{|h_{n-1,n-1}(k)|}{\max\{|h_{n-1,n-1}(k+1)|, \frac{h_{\max}(k+1)}{\gamma} \}} & \text{otherwise.} \end{cases}
\]

Cases $r < n - 1$: Let $A = \max\{|h_{r,r}(k)|, \frac{h_{\max}(k)}{\gamma} \}$ and $B = \max\{|h_{r+1,r+1}(k)|, \frac{h_{\max}(k)}{\gamma} \}$.

Set $\eta = h_{r,r}(k)$, $\lambda = h_{r+1,r+1}(k)$, $\beta = h_{r+1,r}(k)$ and $\delta = \sqrt{\beta^2 + \lambda^2}$. Noticing that $h_{\max}(k) \geq h_{\max}(k+1)$ and $|\eta| > \frac{h_{\max}(k)}{\gamma}$ yields

\[
A = \max\{|h_{r,r}(k)|, \frac{h_{\max}(k)}{\gamma} \} = \frac{|\eta|}{\max\{|h_{r,r}(k+1)|, \frac{h_{\max}(k+1)}{\gamma} \}} = \begin{cases} \frac{|\eta|}{\frac{h_{\max}(k+1)}{\gamma}} & \text{when } \frac{|\eta|}{\frac{h_{\max}(k+1)}{\gamma}} \geq \tau \\ \frac{|\eta|}{\max\{|h_{r,r}(k+1)|, \frac{h_{\max}(k+1)}{\gamma} \}} & \text{otherwise.} \end{cases}
\]

And then, we consider $AB = A \cdot \max\{|\lambda|, \frac{h_{\max}(k)}{\gamma} \}$. When $|\lambda| \geq \frac{h_{\max}(k)}{\gamma}$, it is easily deduced that $\delta \geq |\lambda| \geq \frac{h_{\max}(k)}{\gamma}$ and $\frac{|\eta|}{\delta} > \lambda \geq \frac{h_{\max}(k+1)}{\gamma}$. Hence from equation (B.1) it holds that

\[
AB = A \cdot \frac{|\lambda|}{|\eta|} = A \cdot \frac{\delta}{|\eta|} \cdot \frac{|\eta|}{\delta} = 1
\]

When $|\lambda| < \frac{h_{\max}(k)}{\gamma}$, it holds that

\[
AB = A \cdot \frac{h_{\max}(k)}{\gamma} = \begin{cases} A \cdot \frac{h_{\max}(k)}{\gamma} & \text{when } \frac{|\eta|}{\delta} \geq A \geq \frac{\delta}{|\lambda|} \geq 1 \\ A \cdot \frac{h_{\max}(k)}{\gamma} & \text{when } \frac{|\eta|}{\delta} < A \geq \frac{\delta}{|\lambda|} \geq 1 \end{cases}
\]

Up to now, we have shown that $AB \geq 1$. Therefore

\[
\frac{\Pi(k)}{\Pi(k + 1)} = A[AB]^{n-r-1} > A > \tau
\]
It is proved that

\[(B.2) \quad \left( \frac{h_{\text{max}}(k)}{\gamma^{n-1}} \right)^{\frac{n(n-1)}{2}} \leq \Pi(k) \leq \frac{1}{\tau^k}.\]

From \(\tau > 1\), we have

\[k \leq \frac{n(n-1)((n-1)\log \gamma + \log \frac{1}{h_{\text{max}}(k)})}{2 \log \tau}.\]

From \(|h_{n,n-1}(k)| < |h_{n-1,n-1}(k)| < h_{\text{max}}(k)|\), it always holds that \(h_{\text{max}}(k) \geq \varepsilon_2\) before termination. Hence, we deduce that

\[k \leq \frac{n(n-1)((n-1)\log \gamma + \log \frac{1}{\varepsilon_2})}{2 \log \tau},\]

which completes the proof.

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