A gentle introduction to PSLQ

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Abstract

This is work in progress. Please let me know about any comments and suggestions.

1 What PSLQ is about

PSLQ is an algorithm for finding integer relations. Namely, given n real numbers $\boldsymbol{x} = (x_1, x_2, \ldots, x_n)$ PSLQ tries to find integers $\boldsymbol{m} = (m_1, m_2, \ldots, m_n)$, not all zero, such that

$$\boldsymbol{x} \cdot \boldsymbol{m} = m_1 x_1 + \ldots + m_n x_n = 0.$$

The vector $\boldsymbol{m}$ is called an integer relation for $\boldsymbol{x}$. In case that no relation is found, PSLQ provides a lower bound for the norm of any potential integer relation.

Example 1. Assume the first digits of some real number a have been computed numerically. Based on some theory or educated suspicion one has the hunch that x is a (rational) linear combination of constants $c_1, \ldots, c_n$. PSLQ applied to $\boldsymbol{x} = (a, c_1, \ldots, c_n)$ will substantiate or refute this guess. In particular, PSLQ will provide (candidates for) the coefficients of the seeked linear combination.

Example 2. The Bailey-Borwein-Plouffe formula

$$\pi = \sum_{n=0}^{\infty} \frac{1}{16^n} \left(\frac{4}{8n+1} - \frac{2}{8n+4} - \frac{1}{8n+5} - \frac{1}{8n+6} \right)$$

can be found by using PSLQ applied to $\boldsymbol{x} = (\pi, x_1, \ldots, x_7)$ where

$$x_j = \sum_{n=0}^{\infty} \frac{1}{16^n (8n+j)}.$$

This identity is quite famous, in particular, because it is the basis for an algorithm to compute hexadecimal digits of π without computing previous ones.

By the way, the name PSLQ pertains to partial sums and the LQ decomposition, both of which appear in the outline of the algorithm presented in the sequel.

Our presentation is strongly based on [FBA99]; also see [BB01], and [BL00].

2 Outlining the algorithm

2.1 The basic idea

Let $\boldsymbol{x}=(x_1,x_2,\ldots,x_n)$ be a vector of real numbers. We will assume that $|\boldsymbol{x}|=1$. Define the partial sums

$$s_k^2 := \sum_{j=k}^{n} x_j^2,$$

and construct the $n\times(n-1)$ matrix

$$H_{\boldsymbol{x}} = \begin{pmatrix} \frac{s_2}{s_1} & & & \\ -\frac{x_1x_2}{s_1s_2} & \frac{s_3}{s_2} & & \\ -\frac{x_1x_3}{s_1s_2} & -\frac{x_2x_3}{s_2s_3} & \ddots & \\ \vdots & \vdots & \ddots & \frac{s_n}{s_{n-1}} \\ -\frac{x_1x_n}{s_1s_2} & -\frac{x_2x_n}{s_2s_3} & \cdots & -\frac{x_{n-1}x_n}{s_{n-1}s_n} \end{pmatrix}. \tag{1}$$

Exercise 1. The $n-1$ columns of $H_{\boldsymbol{x}}$ are orthogonal. Furthermore, they are orthogonal to $\boldsymbol{x}$ and therefore form a basis for the relations of $\boldsymbol{x}$. Check this!

The crucial result, see [FBA99, Theorem 1], is the following. Let A be any invertible integer matrix. If Q is an orthogonal matrix such that $AH_{\boldsymbol{x}}Q=L$ is lower trapezoidal (that is LQ^T is the LQ factorization of $AH_{\boldsymbol{x}}$) then

$$|\boldsymbol{m}| \geqslant \frac{1}{\max_j |L_{jj}|} \tag{2}$$

for any integer relation $\boldsymbol{m}$.

Based on this, the strategy of PSLQ is to iteratively produce matrices A and Q such that the above bound (2) is improved at each step until a relation is found or precision is exhausted. Suppose that at some iteration PSLQ has produced $H=AH_{\boldsymbol{x}}Q$. For the next step, PSLQ tries to find an integer matrix D such that DH is “as diagonal as possible while preserving the diagonal” and replaces A by DA. Next, to be able to keep going in this fashion, the matrices A and Q are “slightly perturbed” (namely, two rows of A are exchanged while Q is accordingly modified to keep $AH_{\boldsymbol{x}}Q$ lower trapezoidal). The matrix D is called the Hermite reducing matrix of H and is introduced in the next section.

2.2 Hermite reduction

Given a lower trapezoidal $n\times m$ matrix H with nonzero diagonal elements there is a unique $n\times n$ matrix D_0 such that D_0H is diagonal with the same entries as H on the diagonal. D_0 may be explicitely given by

$$(D_0)_{ij} = \begin{cases} 0 & \text{if } i<j, \\ 1 & \text{if } i=j, \\ -\frac{1}{h_{jj}}\sum_{k=j+1}^{i} (D_0)_{ik}H_{kj} & \text{if } i>j. \end{cases}$$

Exercise 2. Check that $D_0 H$ is indeed diagonal!

Similarly, the $n\times n$ integer matrix D is defined as

$$D_{ij} = \begin{cases} 0 & \text{if } i<j,\\ 1 & \text{if } i=j,\\ \left[-\frac{1}{h_{jj}}\sum_{k=j+1}^{i} D_{ik}H_{kj}\right] & \text{if } i>j,\end{cases}$$

where $[x] = \lfloor x+1/2\rfloor$ denotes rounding to the nearest integer. D is called the Hermite reducing matrix for H, and DH is the Hermite reduction of H.

Remark 3. While DH won't be diagonal in general we still have the estimate

$$|(DH)_{ij}| \leqslant \frac{1}{2}|H_{jj}|$$

for $i\neq j$, see [FBA99, Lemma 4].

2.3 The algorithm

Let $\gamma > 2/\sqrt{3}$. This parameter may be freely chosen.

Initial setup.
Let $H_{\boldsymbol{x}}$ be the matrix defined in (1), and set A to be the Hermite reducing matrix of $H_{\boldsymbol{x}}$. Let Q be the identity matrix.

Step 1: Exchange.
Let r be such that $\gamma^j|(AH_{\boldsymbol{x}}Q)_{jj}|$ is maximal for $j=r$. Exchange rows r and $r+1$ of A. If $r=n-1$ then go to Step 3. Otherwise, $AH_{\boldsymbol{x}}Q$ is no longer lower trapezoidal. This is rectified in the next step.

Step 2: Corner.
Let P be the $(n-1)\times(n-1)$ orthogonal matrix defined by

$$P_{ij} = \begin{cases} a/d & \text{if } i=j=r,r+1,\\ b/d & \text{if } i=r+1,\ j=r,\\ -b/d & \text{if } i=r,\ j=r+1,\\ 1 & \text{if } i=j\neq r,r+1,\\ 0 & \text{otherwise,}\end{cases}$$

where

$$a = (AH_{\boldsymbol{x}}Q)_{r,r},\quad b = (AH_{\boldsymbol{x}}Q)_{r,r+1},\quad d=\sqrt{a^2+b^2}.$$

Replace Q by QP.

Step 3: Reduction.
Let D be the Hermite reducing matrix of $AH_{\boldsymbol{x}}Q$. Replace A by DA.

Step 4: Termination.

If $\boldsymbol{x}\, A^{-1}$ has a zero component then we have found a relation $\boldsymbol{m}$ as the corresponding column of the integer matrix A^{-1}.

Otherwise go back to Step 1. (We keep our spirits up by noting that, by (2), we have already established the lower bound $|\boldsymbol{m}| \geqslant 1/\max_j ((A H_{\boldsymbol{x}}\, Q)_{jj})$.)

Remark 4. If naively implemented the above algorithm performs very poorly and often looses precision too quick to recover a relation. To alleviate this one needs to keep track of the matrices A, A^{-1} and $A H_{\boldsymbol{x}}\, Q$ during the execution of the algorithm. One may also perform the ocurring matrix multiplications inline (that is, for instance, without explicitly constructing the matrix P in Step 2). See [FBA99] for this and [BB01] for spectacular further improvements.

Remark 5. If $A H_{\boldsymbol{x}}\, Q$ has a zero on its diagonal then this must occur, see [FBA99, Lemma 5], for $(A H_{\boldsymbol{x}}\, Q)_{n-1,n-1} = 0$ and it follows that $\boldsymbol{x}\, A^{-1}$ has a zero component. Step 3 may thus always be performed.

Remark 6. To find a relation for $\boldsymbol{x} = (x_1, \ldots, x_n)$ with coefficients of size up to 10^m one needs, as a rule of thumb, somewhat more than nm digits of precision.

Exercise 3. Monitor the behaviour of the quotient of the minimum divided by the maximum modulus of $\boldsymbol{x}A^{-1}$ during the execution of PSLQ.

Exercise 4. Experiment with the choice of the parameter γ. In particular, monitor number of iterations and precision needed depending on γ.

3 Applications

Finally, we present a few applications of PSLQ in the form of exercises. Many more applications may be found for instance in [BL00].

Exercise 5. An algebraic number α may be identified by applying PSLQ to $(1, \alpha, \ldots, \alpha^n)$ and increasing n. Why? Use this idea to identify the number

$$\alpha = 3.6502815398728847452\ldots$$

Exercise 6. Think about how PSLQ could be used to find multiplicative relations by taking logarithms and including logarithms of small primes.

Exercise 7. As advertised in [Cha08], PSLQ may also be used to find integer relations between functions by evaluating them at a fixed random point. Use this approach to express $\sin(7x)$ in terms of $\sin(x), \sin^2(x), \ldots, \sin^7(x)$. Observe and generalize!

Exercise 8. PSLQ may not only be used to identify algebraic numbers, as in Exercise 5, but also to provide rigorous evidence for a number to be transcendental (based on the lower bound (2) for the norm of an integer relation obtained at each iteration). Show that if Euler's constant γ is the root of an integer polynomial of degree up to 10 then the norm of the vector of coefficients exceeds 10^{30}. Make similar claims for Catalan's constant

$$G = \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n+1)^2}.$$

Results of this kind strongly suggest that γ and G are not algebraic. However, as of 2009, it is not even known if they are irrational.

References

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