

A Fast Algorithm for Calculation of Thêo1

Ben Lewis

Abstract—Thêo1 is a frequency stability statistic which is similar to the Allan variance but can provide stability estimates at longer averaging factors and with higher confidence. However, the calculation of Thêo1 is significantly slower than the Allan variance, particularly for large data sets, due to a worse computational complexity. A faster algorithm for calculating the 'all- τ ' version of Thêo1 is developed by identifying certain repeated sums and removing them with a recurrence relation. The new algorithm has a reduced computational complexity, equal to that of the Allan variance. Computation time is reduced by orders of magnitude for many datasets. The new, faster algorithm does introduce an error due to accumulated floating point errors in very large datasets. The error can be compensated for by increasing the numerical precision used at critical steps. The new algorithm can also be used to increase the speed of ThêoBr and ThêoH which are more sophisticated statistics derived from Thêo1.

Index Terms-Noise, Stability analysis, Frequency control, Software, Theo1, TheoH.

I. INTRODUCTION

HEN characterising a frequency source, it is necessary to determine the amount and types of noise which determine the frequency stability on different timescales. There are many statistics used for this purpose, one of which is the 'theoretical variance #1' (Thêo1) [1]. Compared to the more commonly used Allan variance, Thêo1 has increased confidence at long averaging times, and can be used to estimate stability up to 50% longer averaging times. Thêo1 is also better able to identify which type of 'power-law' noise is present [2], [3]. These properties have allowed Thêo1 to be used for longrunning experiments where datasets cannot easily be extended [4]. However, Thêo1 is slow to compute for large datasets, as its computational complexity is $\mathcal{O}(N^3)$ for a dataset of N measurements. Similar statistics with $\mathcal{O}(N^3)$ complexity have been reduced to $\mathcal{O}(N^2)$ complexity by the use of an appropriate algorithm [5].

For a series of N time deviation points x_i , each separated by an interval τ_0 , Thêo1 can be defined [1] as

Thêo1
$$(\tau = 1.5k\tau_0, N) = \frac{T_k}{3(N - 2k)(k\tau_0)^2}$$
 (1)

where $0 < k \le (N-1)/2$, the averaging time is τ and

$$T_k = \sum_{i=0}^{N-2k-1} \sum_{\delta=0}^{k-1} \frac{1}{(k-\delta)} [(x_i - x_{i-\delta+k}) + (x_{i+2k} - x_{i+\delta+k})]^2$$
 (2)

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A naive implementation of this definition of Thêo1 will have a complexity of $\mathcal{O}(N^3)$ because there are $\approx N/2$ values of k for which to calculate T_k , each taking $\mathcal{O}(N^2)$ operations due to the nested sum in (2). This can make computation prohibitively expensive for extremely large datasets or in applications requiring low latency, such as measuring the dynamic stability of an oscillator with a high data rate [6].

In some cases it is not necessary to calculate Thêo1 for every value of k, sometimes called an 'all- τ ' calculation, and it may be sufficient to only use k equal to powers of two. However, the more sophisticated statistics ThêoBr and ThêoH [7], which attempt to correct for bias in Thêo1 require the calculation of Thêo1 for all k as a first step. There is a technique called 'fast TheoBr' [8] which increases the speed of this calculation by averaging points within the initial dataset to reduce its size. However, for a fixed amount of averaging, the speed increase is only a constant factor and does not change the $\mathcal{O}(N^3)$ complexity.

II. ALGORITHM

One way to produce a faster algorithm for Thêo1 is to find a recurrence relation between parts of the outer sum, which allows calculation of one term from the next without performing the full inner sum. This is made difficult by the term $1/(k-\delta)$ which forces a different coefficient before each terms as δ is incremented in the inner sum. However, the definition of T_k can be rearranged to move this awkward term outside the inner sum by swapping the order of the sums and using the substitution $v = k - \delta$, so that

$$T_k = \sum_{v=1}^{k} \frac{1}{v} A_{k,v}$$
 (3)

where $A_{k,v}$ is defined by

$$A_{k,v} = \sum_{i=0}^{N-2k-1} (x_i - x_{i+v} + x_{i+2k} - x_{i+2k-v})^2$$
 (4)

$$= \sum_{i=0}^{N-2k-1} (x_i^2 + x_{i+v}^2 + x_{i+2k}^2 + x_{i+2k-v}^2 + 2x_i x_{i+2k} + 2x_{i+v} x_{i+2k-v} - 2x_i x_{i+v} - 2x_i x_{i+2k-v} - 2x_{i+v} x_{i+2k} - 2x_{i+2k} x_{i+2k-v}).$$
(5)

Some of the expanded terms in (5) have similar forms, and can be expressed in terms of new summations $C^{(n)}$, defined

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$$C_j^{(1)} = \sum_{i=0}^{j} x_i^2 \tag{6}$$

$$C_j^{(2)} = \sum_{i=0}^{N-j-1} x_i x_{i+j} \tag{7}$$

$$C_{k,j}^{(3)} = \sum_{i=1}^{N-k-1} x_{i-j} x_{i+j} \tag{8}$$

$$C_{k,j}^{(4)} = \sum_{i=0}^{N-2k-1} x_i x_{i+j} + x_{i+2k} x_{i+2k-j}.$$
 (9)

It can then be shown by substitution that

$$A_{k,v} = C_{N-2k-1}^{(1)} + (C_{N-2k-1+v}^{(1)} - C_{v-1}^{(1)})$$

$$+ (C_{N-1}^{(1)} - C_{2k-1}^{(1)}) + (C_{N-v-1}^{(1)} - C_{2k-v-1}^{(1)})$$

$$+ 2(C_{2k}^{(2)} + C_{k,k-v}^{(3)} - C_{k,v}^{(4)} - C_{k,2k-v}^{(4)}).$$

$$(10)$$

The calculation of T_k from the $C^{(n)}$ can be completed in $\mathcal{O}(N^2)$, so if the $C^{(n)}$ could all be calculated in $\mathcal{O}(N^2)$ then this would reduce the overall complexity of Thêo1 to $\mathcal{O}(N^2)$. For $C^{(1,2)}$ the definition is already $\leq \mathcal{O}(N^2)$, but it can also be achieved for $C^{(3,4)}$ by using a recurrence relation between consecutive terms to avoid the full sum in (8) and (9):

$$C_{k,j}^{(3)} = C_{k-1,j}^{(3)} - x_{k-1-j} x_{k-1+j}$$

$$- x_{N-k-j} x_{N-k+j}$$

$$, j < k$$

(11)

$$C_{k,j}^{(4)} = C_{k-1,j}^{(4)} - x_{2k-2-j}x_{2k-2} , j < 2k-1$$

$$- x_{2k-1-j}x_{2k-1} - x_{N-2k}x_{N-2k+j}$$

$$- x_{N-2k+1}x_{N-2k+1-j}$$
(12)

This allows almost all values of $C^{(3,4)}$ to be calculated in a recursive manner, the remaining values are

$$C_{b,b}^{(3)} = C_{2b}^{(2)} (13)$$

$$C_{k\,2k-1}^{(4)} = 2C_{2k-1}^{(2)} - x_0 x_{2k-1} - x_{N-2k} x_{N-1} \tag{14}$$

$$C_{k,k}^{(3)} = C_{2k}^{(2)}$$

$$C_{k,2k-1}^{(4)} = 2C_{2k-1}^{(2)} - x_0 x_{2k-1} - x_{N-2k} x_{N-1}$$

$$C_{k,2k}^{(4)} = 2C_{2k}^{(2)}$$

$$(13)$$

$$(14)$$

$$(14)$$

$$(15)$$

and so $C^{(3,4)}$ can be calculated in the required $\mathcal{O}(N^2)$. Because the recurrence relations are for an incremented kvalue, the technique can only be used when calculating T_k for all values of k.

In order to calculate T_k it is sufficient to calculate

$$C_j^{(1)}, \quad 0 \le j \le N$$
 (16)
 $C_j^{(2)}, \quad j = 2k, 2k - 1$ (17)

$$C_j^{(2)}, \quad j = 2k, 2k - 1$$
 (17)

$$C_{k,j}^{(3)}, \quad 0 \le j \le k$$
 (18)

$$C_{k,j}^{(4)}, \quad 0 \le j \le 2k$$
 (19)

so only these values need to be held in memory. The recursion relations (11) and (12) can then be used to update $C_{k,j}^{(3,4)}$ to

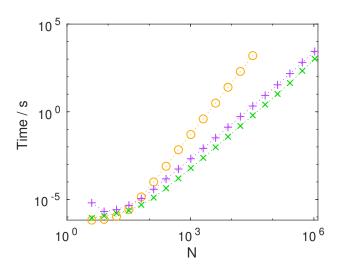


Fig. 1. The time taken by different methods of calculating Thêo1. Orange circles show the naive method. Green 'x' marks show the new algorithm using a standard double precision floating point datatype. Purple '+' marks show the new algorithm using the int-128 datatype.

 $C_{k+1,j}^{(3,4)}$ in place, allowing calculation of T_{k+1} . The memory requirement is only $\mathcal{O}(N)$. Specifically, it requires memory for 4N double precision values: N values for each of the input array x and $C^{(1,4)}$, and N/2 values for each of $C^{(3)}$ and the output array. The naive algorithm requires storage of 3N/2values so this is a significant increase but is still only 32 MB for a dataset with $N = 10^6$.

In order to calculate Thêo1, the algorithm can proceed as follows:

- 1) Calculate $C^{(1)}$ using (6).
- 2) For each value of k from 0 to $\lfloor (N-1)/2 \rfloor$:
 - a) Calculate required values of $C^{(2)}$ using (7).
 - b) Add new values to $C^{(3,4)}$ using (13) to (15).
 - c) Update $C^{(3,4)}$ using (11) and (12).
 - d) Calculate $A_{k,v}$ from the $C^{(n)}$ using (10).
 - e) Calculate T_k from $A_{k,v}$ using (3).

An example implementation of the algorithm in C++ can be found in appendix A.

III. ACCURACY

Whilst the new algorithm for Thêo1 is faster than the naive approach, it has more opportunities for floating point errors to accumulate. Equation (10) shows that terms of similar magnitude are subtracted from each other, allowing catastrophic cancellation to occur and leading to a loss of precision. The size of each term in (10) is $\leq \sum x^2$ and the size of the total is $\sim T_k$, so the fractional error might be expected to scale as $\sim \langle x^2 \rangle / T_k$. Theo is insensitive to any offset or linear change in x, so these components can be removed in order to reduce $\langle x^2 \rangle$ without ill-effect. This prevents a significant drop in precision that could be caused by a constant frequency or phase offset This change alone is sufficient to prevent appreciable errors in most practical situations. However, in some cases with large datasets and where the long-term clock stability is dominated by frequency drift the errors could grow large enough to be significant.

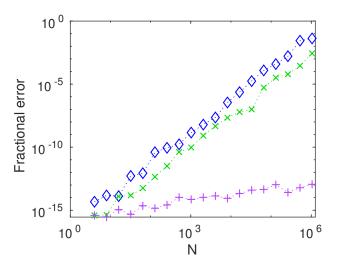


Fig. 2. The maximum fractional error introduced by different methods of calculating Thêo1, measured against the naive method. Green 'x' marks (blue diamonds) indicate the standard double precision method with (without) any linear component removed. Purple '+' marks used the int-128 datatype for increased accuracy. Results depend strongly on the type of noise simulated, for this test white frequency noise with a linear frequency drift was used.

In order to fully mitigate the floating point error it is necessary to use additional bits of precision. Whilst 128-bit floating point types are available in some environments, they are not generally supported in hardware and are therefore very slow to use. In contrast, many 64-bit CPUs have hardware support for multiplying two 64-bit integers into a 128-bit integer. By re-scaling the data and converting it to a 64-bit integer representation, this CPU instruction can be used to calculate Thêo1 quickly without floating point errors. Terms $\propto x$ are stored as 64-bit integers, but terms $\propto x^2$ are stored as 128-bit integers. In C or C++ the GCC __int128 datatype may be used with multiplications implemented as

```
int64_t x1,x2;
__int128 result = (__int128) x1 * x2;
```

The use of a larger data types does cause a speed reduction of approximately 70%, possibly due to additional memory overhead. The conversion between datatypes is $\mathcal{O}(N)$ and takes negligible time in most cases.

The speed and fractional floating point error for the different methods are shown in Figs. 1 and 2 respectively. The fractional error was measured by comparing the value of Thêo1 as calculated with the new algorithm to that calculated with the naive algorithm. Due to the slow speed of the naive algorithm, only points spaced at powers of two were compared, and the maximum of these errors was taken. Fig. 2 should be taken as indicative only as the details vary significantly depending on the noise type of the simulated data, although the 'int-128' method had negligible error in all cases tested. To exaggerate the errors seen, a white frequency noise with added linear frequency drift was simulated. The linear drift was chosen such that the frequency stability at the longest and shortest averaging factors was approximately equal. A linear frequency drift is particularly difficult for the simpler error reduction method (removing any linear component to x) to deal with,

as the dominant x component is quadratic. Despite this, 1 to 2 orders of magnitude improvement was seen.

IV. CONCLUSION

Manipulating the definition of Thêo1 has led to an algorithm that calculates the 'all- τ ' version with a reduced computational complexity of $\mathcal{O}(N^2)$. Although the new algorithm initially lead to loss of precision, this is reduced by removing any linear component in the dataset. In the cases where the error is still significant, it is made negligible by using an int-128 datatype, at the cost of a $\approx 70\%$ slowdown.

This algorithm makes the speed of Thêo1 (and ThêoBr or ThêoH) calculations similar to other time-domain stability statistics such as the Allan variance. The new algorithm can more easily be used in low-latency applications such as characterising oscillators using a high sample rate, and commercial testing of oscillators and other sensors. It also makes the use of dynamic Thêo statistics easier, with opportunities for calculating statistics over multiple timescales simultaneously. Further work could incorporate this algorithm into a dynamic Thêo algorithm and be used to identify changes to clock stability in real-time.

All data and code supporting this publication are openly available from the University of Strathclyde Knowledge-Base at https://doi.org/10.15129/4403d30e-4257-4a4a-817f-f459e7465011.

APPENDIX A EXAMPLE IMPLEMENTATION

```
* Calculates Theol of a given dataset.
* The dataset is assumed to be phase
 data, taken at unit time increments.
 Any linear component to the dataset is
 removed as a first step. Should be
 compiled with -O3 -ffast-math.
 X = input dataset
 N = number of elements in X
 T = Theoloutput
* Ben Lewis, University of Strathclyde
/* Remove any linear part of the dataset */
void removeLinear (double * X, int N) {
    double midpoint = ((double) (N-1))/2;
    long double sum1 = 0;
   long double sum2 = 0;
    for(int i = 0; i < N; i++)
       sum1 += X[i];
       sum2 += X[i]*(i-midpoint);
    double a = sum1/N;
    double b = sum2/N*12/((double)N*N-1);
```

```
4
```

```
for(int i = 0; i < N; i++)
        X[i] = a + b*(i-midpoint);
}
/* The computational routine */
void Theo1 (double *X, double *T, int N){
// Initialise arrays
int k_max = (N-1)/2;
double * C1 = new double [N];
double* C3 = new double[k_max+1];
double * C4 = new double[k_max * 2];
// Preprocess by removing linear part
removeLinear(X,N);
// Calculate C1
double s=0:
for(int i = 0; i < N; i++)
  s += (X[i]*X[i]);
  C1[i] = s;
// Main loop
C3[0] = C1[N-1];
for (int k=1; k \le k_max; k++)
  // Calculate C2 values
  double C2_2k = 0;
  double C2_2k_1 = 0;
  for (int j = 0; j \le N-2*k-1; j++)
    C2_2k += (X[j]*X[j+2*k]);
    C2_2k_1 += (X[j]*X[j+2*k-1]);
  C2 2k 1 += (X[N-2*k]*X[N-1]);
  // Update C3, C4 in place
  for (int v=0; v < k; v++)
    C3[v] = (X[k-1-v]*X[k-1+v])
           + (X[N-k+v]*X[N-k-v]);
  for (int v = 1; v \le 2*k - 2; v + +)
   C4[v-1] = (X[2*k-1-v]*X[2*k-1])
             + (X[2*k-2-v]*X[2*k-2])
             + (X[N-2*k]*X[N-2*k+v])
             + (X[N-2*k+1]*X[N-2*k+1+v]);
 C3[k] = C2_2k;
 C4[2*k-2] = 2*C2_2k_1 - (X[0]*X[2*k-1])
            -(X[N-2*k]*X[N-1]);
 C4[2*k-1] = 2*C2_2k;
  // Calculate un-normalised T_k from C1-C4
  double T k = 0;
  double A0 = C1[N-1] - C1[2*k-1]
            + C1[N-2*k-1] + 2*C2 2k;
  for(int v = 1; v \le k; v++)
    double A1 = A0 - C1[v-1]
              + C1[N-1-v] - C1[2*k-v-1]
              + C1[N-1-2*k+v];
    double A2 = C3[k-v] - C4[v-1]
              - C4[2*k-v-1];
    T_k += (A1+2*A2)/v;
```

```
// Apply normalisation to get Theol T[k-1] = (T_k/(3*(\textbf{double})(N-2*k)*k*k)); } // Release memory \textbf{delete[] C1;} \\ \textbf{delete[] C3;} \\ \textbf{delete[] C4;} \\ \}
```

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REFERENCES

- [1] D. A. Howe and T. K. Peppler, "Very long-term frequency stability: estimation using a special-purpose statistic," in *IEEE International Frequency Control Symposium and PDA Exhibition Jointly with the 17th European Frequency and Time Forum, 2003. Proceedings of the 2003*, May 2003, pp. 233–238.
- [2] J. A. Mcgee and D. A. Howe, "TheoH and allan deviation as power-law noise estimators," *IEEE Transactions on Ultrasonics, Ferroelectrics, and Frequency Control*, vol. 54, no. 2, pp. 448–452, 2007.
- [3] P. D. D. Schwindt, Y. Jau, H. L. Partner, D. K. Serkland, A. Ison, A. McCants, E. Winrow, J. Prestage, J. Kellogg, N. Yu, C. D. Boschen, I. Kosvin, D. Mailloux, D. Scherer, C. Nelson, A. Hati, and D. A. Howe, "Miniature trapped-ion frequency standard with 171yb+," in 2015 Joint Conference of the IEEE International Frequency Control Symposium the European Frequency and Time Forum, 2015, pp. 752–757.
- [4] T. E. Parker, S. R. Jefferts, T. P. Heavner, and E. A. Donley, "Operation of the NIST-F1 caesium fountain primary frequency standard with a maser ensemble, including the impact of frequency transfer noise," *Metrologia*, vol. 42, no. 5, pp. 423–430, sep 2005.
- [5] Mingfu Li, Hsin-Min Peng, and Chia-Shu Liao, "Fast computation of time deviation and modified allan deviation for telecommunications clock stability characterization," in *Proceedings International Symposium on Parallel Architectures, Algorithms and Networks. I-SPAN 2000*, 2000, pp. 156–160.
- [6] D. A. Howe, N. Ashby, D. Lirette, A. Hati, and C. Nelson, "Limited live-time measurements of frequency spectra," in 2011 Joint Conference of the IEEE International Frequency Control and the European Frequency and Time Forum (FCS) Proceedings, May 2011, pp. 1–4, iSSN: 1075-6787.
- [7] D. A. Howe, J. McGee-Taylor, and T. Tassett, "ThêoH Bias-removal Method," in 2006 IEEE International Frequency Control Symposium and Exposition, Jun. 2006, pp. 788–792, iSSN: 2327-1914.
- [8] J. A. Taylor and D. A. Howe, "Fast TheoBR: A method for long data set stability analysis," *IEEE Transactions on Ultrasonics, Ferroelectrics,* and Frequency Control, vol. 57, no. 9, pp. 2091–2094, Sep. 2010.



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