



A practical software package for estimating the periodicities in time series by least-squares spectral analysis

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Abstract

The researchers investigate some phenomena by continuously observing physical variables, i.e., time series. Nowadays, the Least-Squares Spectral Analysis (LSSA) technique has been preferred for the analysis of time series to conduct more reliable analysis. This technique uses the least-squares principle to estimate the hidden periodicities in the time series. Based on the previous investigations, LSSA gives more reasonable results in the experimental time series that have disturbing effects such as the datum shifts, linear trend, unequally spaced data and etc. The LSSA method is a unique method that can overcome these problems without pre-processing the original series. However, a practical and user-friendly software package in C programming language is not available for scientific purposes to implement the LSSA method. In this paper, we review the computational scheme of the LSSA method, then a software (LSSASOFT) package in the C programming language is developed in the view of the simplicity of the method and compatibility of all types of data. Finally, LSSASOFT is applied in two sample studies for the determining hidden periods in the synthetic data and sea level observations. Consequently, the numerical results indicate that LSSASOFT is a useful tool that can efficiently predicting hidden periodicity for the experimental time series that have disturbing effects.

1. Introduction

It is customary to analyse the successive observations which are ordered chronologically, i. e., time series. There are two main aims of the time series analysis: (i) understanding the nature of the phenomena represented by the sequence of observations, and (ii) predicting the future from the observed time series variables [1-3].

The spectral analysis of any time series means that the hidden periodicities are determined in the data, particularly, the researchers investigate some phenomena in order to identify the physical processes that cause periodic behaviours. For this purpose, a variety of methods have been recently developed and inter-compared in the literature such as Fourier, singular spectrum, wavelet, and least-squares spectral analysis [3-5].

Occasionally, the time series originating from certain experiments (experimental measurements) have many disturbances that directly affect the analysis. Some disturbing effects are the presence of datum shift, trend, short gap, unequally spaced data, and weighted data in the time series. In practice, several temporary solutions

are performed to overcome these difficulties. For instance, (i) the trend (linear) is removed before the analysis; (ii) if the data includes two or more datum shifts, every datum is analysed separately, which means the disorder of complete analysis; (iii) when the time series have short gaps or unequally spaced data, the gaps or certain values are predicted and filled by using the harmonic analysis or any interpolation technique [5]. The whole solutions discussed above change the spectral content of the time series. Thus, an alternative technique is developed without the corruption of data originality, which is called "Least Squares Spectral Analysis (LSSA)". The previous investigations indicate that the LSSA method gives more reasonable results in the experimental time series, compared with other spectral analysis methods [5-8].

The LSSA method was first invented and published by Petr Vanicek who is one of the most famous geodesists [9,10]. Therefore, this method was also so-called "Vanicek Spectral Analysis" in geodetic literature [11].

Later, Vanicek and his colleagues released an improved version of the method furnished with a primitive FORTRAN codes [12]. Many researchers

successfully applied this technique in some fields, especially, in geodesy and related disciplines such as electronic distance measurement, tidal data, superconducting gravimeter data, star positioning, earth-quake, temperature estimating, and seismic data [4, 13-18]. However, a practical and user-friendly software package in the C programming language is still not publicly available for the scientific communities, although a MATLAB code can be found in the literature [17]. As is known, FORTRAN programming is an old fashion language which is not easily understandable for new generation programmers. Hence, as an alternative, an open-source scientific program is developed in the C platform and presented to global users by adding a new algorithm and some elective options as well as considering the former FORTRAN codes written by [12].

The manuscript begins with a brief review of the computational scheme of the LSSA method in section 2. Then, the software which employs the LSSA approach with the new algorithm is presented and discussed in section 3. Afterwards, the paper is followed by two numerical applications based on the simulated and real data, respectively, in section 4. Finally, a short summary concludes the paper in section 5.

2. Least-squares spectral analysis

This section shortly discusses the general structure of any time series, then, briefly reviews the computational scheme of the LSSA method which is used in the software.

2.1. Basic approach

The LSSA method is an application of the least-squares approach in the spectral analysis of time series. This method utilises the least squares approximation to minimize the norm of the residual vector of the time series by estimating the periodic components as well as non-periodic ones [19].

The empirical time series consist of signal and noise. The noise which is the disturbing effect on the observation is divided into two components: random (white) and systematic (coloured). An ideal noise called "white noise" is uncorrelated with any dependent variable. Nevertheless, in practice, a systematic noise called "coloured noise" occurs and is correlated with one or more variables. Systematic noise can be defined by mathematical functions, but their magnitudes are not known in the time series. It is categorized into two types: periodic and non-periodic. The main aim of the LSSA method is to be able to determine these systematic noises (both periodic and non-periodic) simultaneously [19].

2.2. Mathematical theory

The mathematical background of the spectral analysis can be described as follows;

1. vector of observation time: $t_i, i = 1, 2, \dots, n$
2. vector of observables: $f(t_i)$
3. vector of frequencies for which spectral values are desired: $\omega_j, j = 1, 2, \dots, m$

The $s(\omega_j)$ vector which is the spectral value of the ω_j frequency, is sought by the spectral analysis. There are a wide range of ways of calculating a spectrum from the time series. Here, we simply state the problem in the Least Squares Approximation (LSA). Thus, the time series can be modelled by Equation 1.

$$g = Ax \tag{1}$$

where A is the coefficients matrix designing the mathematical relationship between the vectors of observations and unknown parameters. The elements of the design matrix are summarized by Equation 2:

$$A = \begin{bmatrix} \cos \omega_j t_1 & \sin \omega_j t_1 \\ \cos \omega_j t_2 & \sin \omega_j t_2 \\ \vdots & \vdots \\ \cos \omega_j t_n & \sin \omega_j t_n \end{bmatrix} \tag{2}$$

where n represents maximum number of elements.

For computing these parameters by the least-squares approximation, the square root of differences between f and g functions should be minimum. Using the standard least-squares notation [20], we can write it as (Equation 3).

$$\hat{r} = f - \hat{g} = f - A(A^T P A)^{-1} A^T P f \tag{3}$$

where \hat{r} is the residual vector, \hat{g} is the best approximation of f by the least squares method. A spectral value can be calculated by the ratio (Equation 4),

$$s = \frac{f^T \hat{g}}{f^T f} \tag{4}$$

where T denotes transpose of the matrix.

In the case where the spectral value is desired to compute for a frequency ω_j , the result is calculated by (Equation 5).

$$s(\omega_j) = \frac{f^T \hat{g}(\omega_j)}{f^T f} \tag{5}$$

In the parameter estimation methodology through the least-squares approximation, it is essential important to evaluate the results, statistically. Therefore, another great advantage of the LSSA method is that the significance of peaks in the spectrum can be tested statistically in a rigorous manner, which is called confidence level.

Pagiatakis [21] introduces a test as follows: a statistical test of null hypothesis $H_0 : s(\omega_j) = 0$ can be tested with a decision function by Equation 6.

$$s(\omega_j) \begin{cases} < (1 + (\alpha^{-2m/v} - 1)^{-1})^{-1} ; \text{accept } H_0 \\ > (1 + (\alpha^{-2m/v} - 1)^{-1})^{-1} ; \text{reject } H_0 \end{cases} \tag{6}$$

where α is the significance level (usually 5%), m is the number of frequencies participated in simultaneously estimation of the LSSA, v is the degree of freedom.

2.3 LSSA with the known constituents

For some applications, it is known that there are some constituents (e. g. datum shift) in the time series. In this case, we should know something about constituents to deal with them more efficiently. In other words, we know the type of base functions $\phi_i(t)$, but do not need to know the magnitudes of the constituents in the experimental time series. Hence, it is given by Equation 7.

$$f(t) = \sum_i^{NK} c_i \phi_i(t) \quad (7)$$

where NK is the number of known constituents, c_i are the unknown parameters. We know all the $\phi_i(t)$, but not the coefficients c_i in any time series. Thus, the design (coefficients) matrix can be divided into the known constituents and spectral functions ($\cos \omega_j, \sin \omega_j$). The design matrix A can be extended as follows (Equation 8).

$$A = \begin{bmatrix} \phi_1 & \phi_2 & \dots & \phi_{NK} & \cos \omega_j t_1 & \sin \omega_j t_1 \\ \phi_1 & \phi_2 & \dots & \phi_{NK} & \cos \omega_j t_2 & \sin \omega_j t_2 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ \phi_1 & \phi_2 & \dots & \phi_{NK} & \cos \omega_j t_n & \sin \omega_j t_n \end{bmatrix} \quad (8)$$

Thereby, the known constituents are not necessary to be removed from f before the evaluation of the spectrum [10].

Accordingly, three types of known constituents are inserted into the software. [12] explains their base functions in detail. They are concisely reviewed as follows:

- datum bias ($\phi(t) = 1$): For example, a tide gauge is moved to other places a few times during the sea level observations. The dates of the movement are well-documented, but the vertical relationship of the movement is not reported properly.
- linear trend ($\phi(t) = t$): For example, the dock where a tide gauge is located, is slowly sinking into the seabed. Another reason may be that the mean sea level is rising due to global warming.
- forced period ($\phi_1(t) = \cos \mu t$ and $\phi_2(t) = \sin \mu t$). For example, it is known that the time series consists of some frequencies, so we desire to remove these frequencies from the series and to analyse what is remained.

The known constituents mentioned above can be modelled and removed from the given time series simultaneously, then, the residual time series is examined by the LSSA method.

3. LSSASOFT: Software for Estimating Periodicities in Time Series

This section is dedicated to providing a comprehensive explanation of the structure of the software, named 'Least Squares Spectral Analysis SOFTWARE (LSSASOFT),' which is encoded in the C++ platform. Furthermore, the author has rigorously

integrated a new approach into the software to accelerate the LSSA procedures.

3.1 Functions of the software

The LSSASOFT comprises a main function and four sub-functions (subroutines): SPEC, BASE, CHLS, and HELP. Below are brief descriptions of these functions:

- MAIN function: At first, it takes the data file name and all options from the command line (i.e. console user interfaces). In the data file, every record should include the time and variable, respectively. The program enables the evaluation of the weighted data in the case that the third column should be the weight of the observation. In this case, user do not need to revise the software namely, it directly reads the third column. Afterwards, considering the options and the other parameters, all periodic components obtained from the time series are reflected to the screen sequentially.
- SPEC function: It computes the spectral values of the frequencies determined at the beginning of the MAIN function. Wells et al. [12] introduces two algorithms that estimate the spectral values: the first is for equally spaced data and the other is for unequally spaced data. The algorithm for unequally spaced data covers that for equally spaced data. Nevertheless, the algorithm for equally spaced data is faster than the other with respect to the computation time [12]. In the current software, the algorithm for unequally spaced data was preferred by considering the advances in today's computer technology, because the time differences between two algorithms can be comfortably neglected.
- BASE function: It calculates the functional values of the known constituents stated in the user's options. This function concerns three types of known constituents, i. e., the datum bias, linear trend, and forced period. Indeed, the type of known constituent in the time series may be more than three, in this case, the interested users can easily adopt a new constituent (e. g. an exponential trend) according to their experiences.
- CHLS function: It computes the inversion of the normal equation matrix through the use of Cholesky decomposition. Cholesky decomposition is integrated into LSSASOFT due to its compatibility with symmetric and positive-definite matrices. Interested readers can replace the function with a more efficient algorithm such as the LU (Lower-Upper) decomposition.
- HELP function: It offers an overview of the software. When you input the '-h' option or unexpected options, the HELP function becomes active. It elaborates on how LSSASOFT functions alongside different options and outlines the necessary parameters for each option.

3.2 New algorithm

In order to expedite the computational procedures of the LSSA method, a new algorithm designed by the

author is adapted to the LSSASOFT. This algorithm automatically enables the determination of the periods in the time series.

The normal procedure of the LSSA method is following: firstly, the time series and its constituents (linear trend, datum shifts, and forced periods) are read from the data and options files, then the spectral values of the whole frequencies determined by the user are computed, finally, the peaks over the confidence level are manually determined as indicators of the periodicities. Every periodicity determined in the previous step is sequentially suppressed by adding it to a forced period for the purpose of detecting other un-catched periodicities manually [22]. Moreover, the user should know the approximate spectral band to determine the periodicities very well, which means that analyst should be expert on the subject. These procedures are time consuming and laborious tasks for the analysts to get reliable results.

Considering all these limitations, a new algorithm was developed in this study as:

1. start,
2. get the parameters from the command line (LT: linear trend, NDAT: number of datum bias, DAT: times of datum bias, NPER: number of forced periods, PER: forced periods), and read the data file (f(t)),
3. produce all periods (P) ranging from 0.5 (corresponding to the nyquistik frequency) and N/2 (the half-length of the data),
4. compute the spectral value of every period (S(P)) increased by δt ,
5. determine the period (p) corresponding to the highest spectral value (S_{max}),
6. if this spectral value is lower than the confidence level (CL), exit to the program successfully.
7. otherwise, zoom this period (p) by giving ± 1 to the interval, i. e., the new spectral band is ranging from $p - 1$ to $p + 1$ in order to determine the period more precisely,
8. compute the spectral values of all periods in the new interval,
9. promote the period whose spectral value is the highest in all, to the forced period, and print to screen,
10. return to item 3.

The flow chart of the algorithm is pictured in Figure 1. In order to assess the performance of this algorithm, two example applications are done in the next section. The data files are provided together with the program in the case that the user re-simulates the results and checks the implementations.

4. Numerical applications

In order to exemplify the capabilities of the LSSASOFT and the usefulness of the new algorithm in the studies, two representative sample data were analysed separately. In the first example, we used synthetic data which comprises 300 records. In the second example, we utilized the hourly sea level observations obtained from the Antalya tide-gauge in 1990, Türkiye. Hence, it was

shown whether the periods estimated by the software are reliable or not.

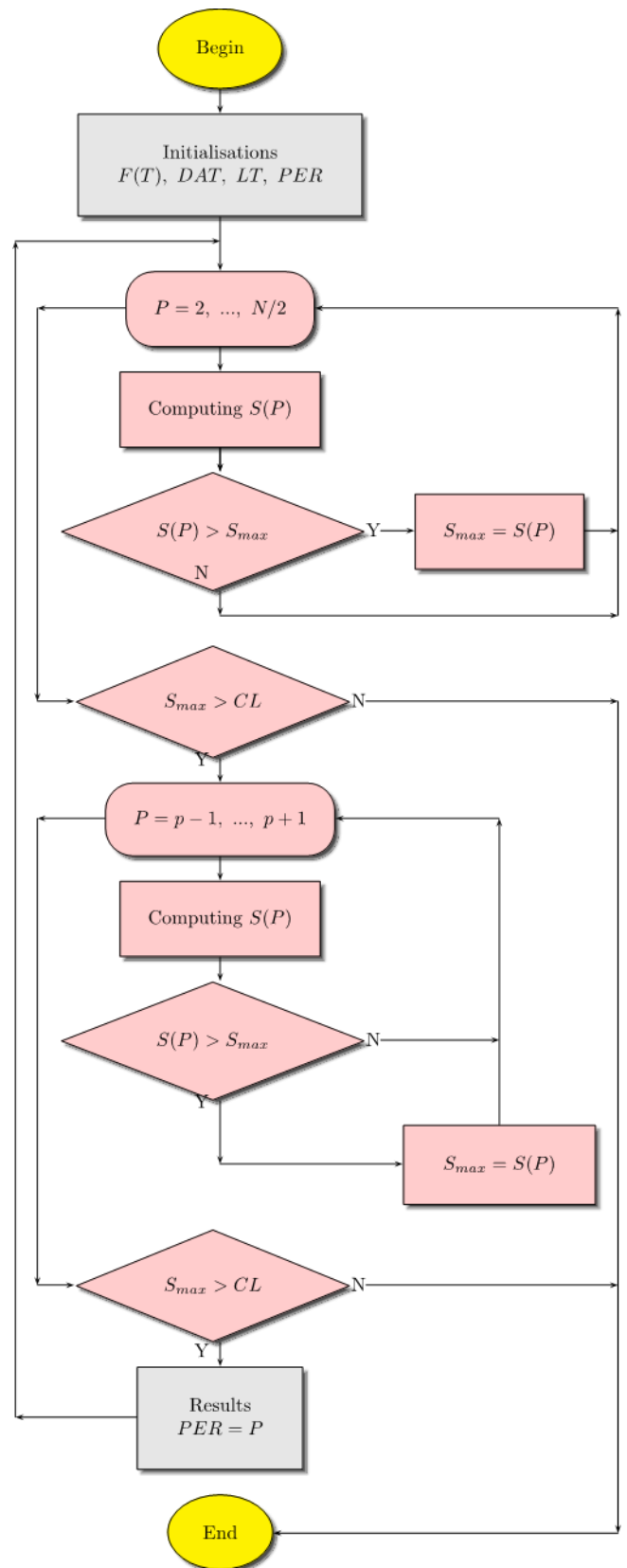


Figure 1. The flow chart of new algorithm added to the software.

4.1 Testing the software on synthetic data

In this example, synthetic data representing a typical

coloured time series, was generated from Equation (9) which is partly used by [12]. This series was equally spaced and equally weighted with no covariance information, subsequently, it was chosen to perform the statistical testing at the 99% confidence level, which is the most rigorous option in geodetic literature.

The mathematical illustration of the test time series is given as:

$$f(t) = c_i + 0.01t + \sum_{j=1}^4 (a_j \cos \mu_j t + b_j \sin \mu_j t) \quad (9)$$

where t is the time (unit: year), c_i is the datum bias, μ_j is the periodic component, a_j and b_j are the coefficients of the periodic components.

Three hundred values of f , which spans 50 years were calculated and grouped into four sub-intervals consisting of equally spaced data, that is

$$t \in D_k, k = 1, 2, 3, 4,$$

where

- $D_1 \equiv [0.1, 0.2, \dots, 10.0]$ years (100 values)
- $D_2 \equiv [20.1, 20.2, \dots, 25.0]$ years (50 values)
- $D_3 \equiv [28.1, 28.2, \dots, 40.0]$ years (120 values).
- $D_4 \equiv [47.1, 47.2, \dots, 50.0]$ years (30 values)

The datum biases are $c_1 = 1.0, t \in D_1; c_2 = -1.0, t \in D_2; c_3 = 3.0, t \in D_3, D_4$. The coefficients of the trigonometric terms are $a_j = 0.5, 1.0, 0.0, -0.25; b_j = 1.0, 0.5, 1.0, 0.0$, respectively. The periods are $p_j = 2\pi/\mu_j = 2.759, 3.636, 5.714, 18.0$ years. Figure 2 displays the behaviour of test series under investigation.

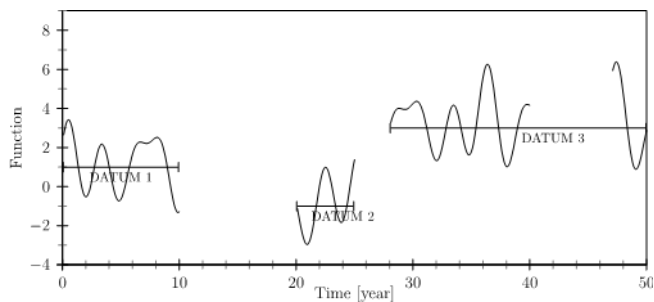


Figure 2. Graph of the test time series.

According to these parameters, the software run with the following options:

```
./LSSASOFT test.dat -d3/0.1/20.1/28.1 -l
```

where the “test.dat” file contains the test time series made of time and value which are available along with the software package; the “d” option denotes the number of datum bias and times of datum biases in sequence; the “l” option means that the time series posses the linear trend. The numerical results from the analysis are listed in Table 1.

According to Table 1, the periodicities in the test series were successfully determined by the LSSASOFT. The differences between the real and estimated values are very small, which is negligible in the numerical analysis.

Table 1. The numerical results from running the LSSASOFT by the first test time series.

Number	Real period	Estimated period	Spectral value	Differences
1	2.759	2.758	94.81	0.001
2	3.636	3.629	44.13	0.007
3	5.714	5.726	43.09	0.012
4	18.00	17.671	52.69	0.329

4.2 Sea level observations

In the second example, we utilized the real sea level observations supplied from the Antalya tide-gauge in 1990 in Türkiye. These observations were selected as test data because they inherently involved all kinds of disturbances due to the fact that the tide-gauge had a classical instrument.

Before the analysis, the general structure of the sea level data should be considered more closely. Accordingly, the sea level observations are decomposed to three components (Equation 10) [23]:

$$\text{Observation} = \text{mean sea level} + \text{tides} + \text{atmospheric residuals} \quad (10)$$

where all components are related with the different physical process and uncorrelated with each other. The mean sea level is determined by averaging hourly data at least 20 years long since the longest period of tidal components is 18.6 years. Accordingly, the tides are the periodic sea level changes that are consistent with some geophysical effects, and are of the certain amplitude and phase [24]. Atmospheric residuals are irregular variations related with weather conditions, which is the so-called “surge effect”.

The tides mentioned above are simply explained by Newton’s gravity force. This force (F) is summarized by (Equation 11).

$$F = -G \frac{m_1 m_2}{r^2} \quad (11)$$

where G denotes the Newtonian gravitation constant, r represents the distance between m_1 and m_2 . Provided that the masses of the Earth and the Moon, and also the distance between the planets are inserted to the equation, the result is the gravitational force between them. The gravitation between the Earth and Sun can be achieved similarly. Both gravitations affect the sea level changes in the same periods with the movements of the Sun and the Moon [25]. Accordingly, tidal components are demonstrated in Table 2.

Table 2. The primary short tidal components [26].

Tidal components	Real Period	Description	Explanation
M2	12.4206	Principal lunar	Semi-diurnal
S2	12.0000	Principal solar	Semi-diurnal
N2	12.6584	Larger Lunar elliptic	Semi-diurnal
K2	11.9673	Luni-solar	Semi-diurnal
K1	23.9344	Luni-solar diurnal	Diurnal
Q1	25.8194	Principal lunar diurnal	Diurnal
P1	24.0659	Principal solar diurnal	Diurnal
Q1	26.8684	Larger Lunar elliptic	Diurnal

Before the numerical analysis of our sea level observation, the observations were plotted month by month. While the observations are examined carefully, it is clear that there is a variety of difficulties (e. g. gappy data, linear trend) in the time series (Figure 3).

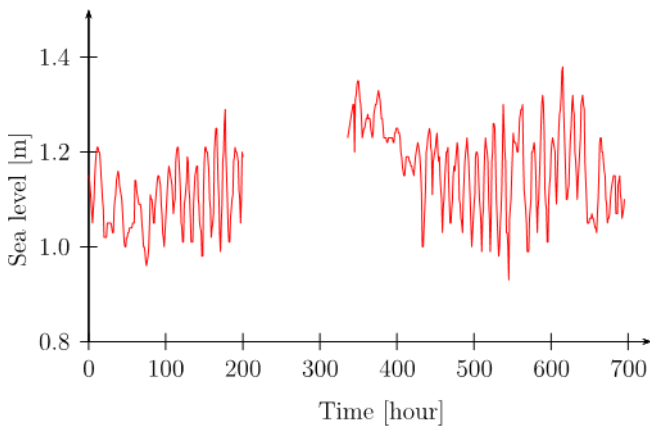


Figure 3. A sample data from the Antalya tide gauge (April 1990).

The hourly sea level data obtained from every month was analysed in a sequence. As a result of this analysis, two dominant periods were successfully estimated in the sea level observations (Table 3). Unfortunately, others are not determined due to the data length (i. e. one month long).

Table 3. The numerical results from the running the LSSASOFT by the sea level series.

Month	Period 1	Period 2
January	11.998	12.416
February	12.009	12.437
March	11.957	12.393
May	11.860	12.337
June	12.325	12.386
July	11.987	12.405
August	11.987	12.418
September	11.971	12.393
October	11.982	12.405
November	12.048	12.447
December		12.418
Average	12.013	12.412
Std.	0.11	0.037

In order to check whether the results are compatible with astronomical counterparts, a test was carried out by using the student distribution (t test). A statistical test of null hypothesis $H_0: \bar{x} = \mu_0$ can be tested through a decision function by Equation 12.

$$t_{test} = \frac{|\bar{x} - \mu_0|}{\sigma_x / \sqrt{n}} \begin{cases} \leq t_{\alpha, f} & ; \text{accept } H_0 \\ > t_{\alpha, f} & ; \text{reject } H_0 \end{cases} \quad (12)$$

where α is the significance level (5%), f is the degree of freedom, σ_x is the standard deviation of the periodicity, \bar{x} denotes the average value of the periodicity, μ_0 represents the astronomical value of the periodicity.

As a result of the test, all periods derived from the analysis are well-consistent with the astronomical

counterparts at a confidence level of 95%. This result indicates that the software is successful on the determination of the hidden periodicity in the time series induced by the disturbing effects.

Although there are totally eight diurnal and semi-diurnal tidal components, two of them could be determined by using the program in the current study, which are compatible with a previous study done by FORTRAN codes [27]. The reasons of incomplete frequencies are evaluated that the other components might have low amplitudes, or that the dock structure and geographical position of the tide gauge might be unsuitable to sense the other tidal components.

On the other hand, nowadays the least squares principle has been frequently employed in some geodetic problems such as gravimetric geoid determination [28,29].

4. Conclusion

The present contribution has reviewed the fundamental theory of the LSSA approach to spectral analysis of time series. The LSSA is an efficient method to determine the periodicities in the empirical time series that have difficulties. Then, an open-source software package developed according to the mentioned theory of the LSSA approach is presented by adding a new algorithm with a range of elective options. Lastly, the present paper is continued by two numerical applications based on the synthetic and real data, respectively. The numerical analyses point out that the LSSASOFT produces considerably reasonable results in both time series.

The current contribution focuses on the significant computational aspects of the LSSA approach. To determine the best solution for estimating periodicities using LSSASOFT, we strongly encourage interested users to run the software with their data, experiment with various modifications, compare the results, and draw conclusions based on their test results.

From another perspective, the software is intentionally designed to consist of a range of different sub-routines. This structure enables end users to replace their specific sub-routines (e.g., adding an alternative base function and inverse function for normal equation matrix etc.) without adversely affecting the remaining components of LSSASOFT.

As a result, the software is highly structured and user-friendly, making it suitable for academic purposes. We hope that the availability of LSSASOFT will encourage researchers in various scientific fields to apply the LSSA method to their data, including disciplines such as GNSS (Global Navigation Satellite Systems) coordinate time series, which mostly exhibit discontinuities (offsets) and linear trends due to tectonic phenomena.

As a future work, it is noteworthy mentioned here that the extended version of LSSA, such as Least Squares Wavelet Analysis [30] can be also developed in the C programming language. Hence, a rich C/C++ library about spectral analysis may be created for the scientific communities.

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Computer code availability

The current software, developed in the C programming language, is freely available under the GNU General Public License. Interested readers can access the software, along with synthetic and experimental data, on GitHub at www.github.com/aabbak/LSSASOFT. The author welcomes inquiries and bug reports related to the software.

Conflicts of interest

The authors declare no conflicts of interest.

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