

Stochastic significance of peaks in the least-squares spectrum

S. D. Pagiatakis

Natural Resources Canada, Earth Sciences, Geodetic Survey Division, 615 Booth Street, Ottawa, Ontario, Canada K1A 0E9
e-mail: pagiatakis@geod.nrcan.gc.ca; Tel.: 613 995 8720; Fax: 613 992 1468

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Abstract. The least-squares spectral analysis method is reviewed, with emphasis on its remarkable property to accept time series with an associated, fully populated covariance matrix. Two distinct cases for the input covariance matrix are examined: (a) it is known absolutely (a-priori variance factor known); and (b) it is known up to a scale factor (a-priori variance factor unknown), thus the estimated covariance matrix is used. For each case, the probability density function that underlines the least-squares spectrum is derived and criteria for the statistical significance of the least-squares spectral peaks are formulated. It is shown that for short series (up to about 150 values) with an estimated covariance matrix (case b), the spectral peaks must be stronger to be statistically significant than in the case of a known covariance matrix (case a): the shorter the series and the lower the significance level, the higher the difference becomes. For long series (more than about 150 values), case (b) converges to case (a) and the least-squares spectrum follows the *beta distribution*. The results of this investigation are formulated in two new theorems.

Key words. Least squares · Spectrum · Hindcast skill · Regression · Statistical test

1 Introduction

It is customary to expect that the researcher or engineer has to deal with experimental time series with missing data points. Occasionally, time series originating from certain experiments, such as astronomical observations, are inherently unequally spaced, or we may intentionally introduce a variable sampling rate to avoid aliasing. Furthermore, advances in instrument development and our better understanding of the physical phenomena result in improvements in the accuracy of the data.

Thus, time series collected over long periods will be non-stationary by virtue of being unequally weighted. Disturbances originating from instrument replacement or repair may also introduce datum shifts (offsets) in the series.

Fashionable spectral estimation techniques have been related almost entirely to fast Fourier transform (FFT) algorithms for the determination of the power spectrum. The FFT approach is computationally efficient and produces reasonable results for a large class of signal processes (Kay and Marple 1981). However, FFT methods are not a panacea in spectral analysis. There are many inherent limitations, the most prominent being the requirement that the data be equally spaced and equally weighted (e.g. Press et al. 1992). Pre-processing of the data is inevitable in these cases, it is unsatisfactory and it performs poorly (Press and Teukolsky 1988).

Least-squares spectral analysis (LSSA) was first developed by Vaniček (1969, 1971) as an alternative to the classical Fourier methods. LSSA bypasses all inherent limitations of Fourier techniques, such as the requirement that the data be equally spaced (e.g. Press et al. 1992), equally weighted, with no gaps and datum shifts. In Sect. 2, we revisit the LSSA, emphasising its remarkable properties and focusing on the covariance matrix of the input series in order to derive the probability density function underlining the least-squares spectrum (Sect. 5). We distinguish two cases regarding the input covariance matrix: (a) it is known absolutely (a-priori variance factor known); and (b) it is known up to a scale factor (a-priori variance factor unknown), thus the estimated covariance matrix is used. We formulate the criteria for the determination of a threshold value above which the least-squares spectral peaks are statistically significant. It is important to mention that in all of our derivations the covariance matrix is assumed to be fully populated, that is, the time series values need not be statistically independent as it has been postulated in previous studies (e.g. Vaniček 1971; Lomb 1976; Steeves 1981a; Scargle 1982; Press and Teukolsky 1988).

2 Least-squares spectral analysis

2.1 Preliminaries

An observed time series can be considered to be composed of *signal*, a quantity of interest, and *noise*, an unwanted quantity that distorts the signal. The noise can be *random* or *systematic*. An idealised concept of random noise is the *white noise*, which is completely uncorrelated, possessing constant spectral density, and it may or may not follow the Gaussian distribution. In practice we usually deal with *non-white random noise*, a band-limited random function of time. Systematic noise is noise whose form may be describable by a certain functional form; it can be periodic (*coloured*), or non-periodic. Non-periodic noise may include datum shifts (offsets) and trends (linear, quadratic, exponential, etc.), and renders the series *non-stationary*, i.e. it causes the statistical properties of the series to be a function of time.

LSSA (Vaniček 1969, 1971) is an alternative to classical Fourier spectral analysis, for it provides the following advantages: (a) systematic noise (coloured or other) can be rigorously suppressed without producing any shift of the existing spectral peaks (Taylor and Hamilton 1972), (b) time series with unequally spaced values can be analysed without pre-processing (Maul and Yanaway 1978; Press et al. 1992); (c) time series with an associated covariance matrix can be analysed (Steeves 1981a); and (d) statistical testing on the significance of spectral peaks can be performed.

Promising and powerful as it may sound, least-squares spectral analysis has received relatively little attention. It has been applied successfully in its original (Vaniček 1971) or alternate forms by a number of researchers in the field of observational astronomy (e.g. Lomb 1976; Scargle 1982; Press et al. 1992), or in the field of geodetic science (e.g. Maul and Yanaway 1978; Merry and Vaniček 1981; Steeves 1981b; Delikaraoglou 1984; Pagiatakis and Vaniček 1986).

2.2 Mathematical representation of the least-squares spectrum

We consider an observed time series that is represented by $\mathbf{f}(t) \in \mathcal{H}$, where \mathcal{H} is a Hilbert space. The values of the series have been observed at times $t_i, i = 1, 2, \dots, m$; here, we do not assume that t_i are equally spaced. We assume, however, that the values of the time series possess a fully populated covariance matrix \mathbf{C}_f , that metricises \mathcal{H} .

One of the main objectives of LSSA is to detect periodic signals in \mathbf{f} , especially when \mathbf{f} contains both, random and systematic noise. Thus, time series \mathbf{f} can be modelled by \mathbf{g} as follows:

$$\mathbf{g} = \Phi \mathbf{x} \quad (1)$$

where $\Phi = [\Phi_s | \Phi_n]$ is the Vandermonde matrix and $\mathbf{x}^T = [\mathbf{x}_s | \mathbf{x}_n]^T$ is the vector of unknown parameters. Subscripts [s] and [n] refer to the signal and noise, respectively. Matrix Φ specifies the functional form of both signal and (systematic) noise. We must emphasise

here that the distinction between signal and noise is subjective; therefore, the partitioning of Φ and \mathbf{x} is arbitrary. We wish to determine the model parameters, such that the difference between \mathbf{g} and \mathbf{f} (residuals) is minimum in the least-squares sense. Using the standard least-squares notation (e.g. Vaniček and Krakiwsky 1986) we can write

$$\hat{\mathbf{r}} = \mathbf{f} - \hat{\mathbf{g}} = \mathbf{f} - \Phi(\Phi^T \mathbf{C}_f^{-1} \Phi)^{-1} \Phi^T \mathbf{C}_f^{-1} \mathbf{f} \quad (2)$$

In the above equation, $\hat{\mathbf{g}}$ is the orthogonal projection of \mathbf{f} onto the subspace $\mathbf{S} \subset \mathcal{H}$ generated by the column vectors of Φ . It follows from the *projection theorem* (Oden 1979) that $\hat{\mathbf{r}} \perp \hat{\mathbf{g}}$. This means that \mathbf{f} has been decomposed into a signal $\hat{\mathbf{g}}$ and noise $\hat{\mathbf{r}}$ (residual series). Equation (2) describes a linear weighted least-squares regression. A simple (un-weighted) least-squares regression can be found for instance in Preisendorfer (1988 p. 322), with its geometrical interpretation given in Fig. 9.1 of his work (Preisendorfer 1988, p. 324).

In order to find something similar to spectral value, we have to compare $\hat{\mathbf{g}}$ to the original series. This can be achieved by projecting orthogonally $\hat{\mathbf{g}} \in \mathbf{S}$ back onto, \mathcal{H} , and comparing the norm of this projection to the norm of \mathbf{f} . Hence, we can obtain a measure (in terms of percent) of how much of $\hat{\mathbf{g}}$ is contained in \mathbf{f} . This ratio is smaller than unity and can be expressed as follows:

$$s = \frac{\langle \mathbf{f}, \hat{\mathbf{g}} \rangle / \|\mathbf{f}\|}{\|\hat{\mathbf{g}}\|} = \frac{\langle \mathbf{f}, \hat{\mathbf{g}} \rangle}{\|\mathbf{f}\|^2} = \frac{\mathbf{f}^T \mathbf{C}_f^{-1} \hat{\mathbf{g}}}{\mathbf{f}^T \mathbf{C}_f^{-1} \mathbf{f}}, \in (0, 1) \quad (3)$$

where the symbols $\langle \rangle$ signify inner product. It is interesting to note here the equivalence of Eq. (3) to the *regression hindcast skill* as presented by Preisendorfer (1988 p. 334). Using our notation, the hindcast skill S_H of the linear least-squares regression [see Preisendorfer 1988, Eq. (9.48)] is $S_H = \|\hat{\mathbf{g}}\|^2 / \|\mathbf{f}\|^2$. Since $\|\hat{\mathbf{g}}\|^2 = \langle \mathbf{f}, \hat{\mathbf{g}} \rangle^2 / \|\hat{\mathbf{g}}\|^2$, then $S_H = \langle \mathbf{f}, \hat{\mathbf{g}} \rangle / \|\mathbf{f}\|^2 \cdot \langle \mathbf{f}, \hat{\mathbf{g}} \rangle / \|\hat{\mathbf{g}}\|^2 = \langle \mathbf{f}, \hat{\mathbf{g}} \rangle / \|\mathbf{f}\|^2 = s$

So far, we have not specified the form of the signal through base vectors that form Φ . In spectral analysis, it is customary to search for, among others, periodic signals that are expressible in terms of sine and cosine base functions. Thus, we can assume a set of spectral frequencies $\Omega = \{\omega_i; i = 1, 2, \dots, k\}$, each defining a different subspace \mathbf{S} spanned by Φ (Wells et al. 1985)

$$\Phi = [\cos \omega_i t, \sin \omega_i t], \quad i = 1, 2, \dots, k \quad (4)$$

and the orthogonal projection of \mathbf{f} onto \mathbf{S} will be different for each $\omega_i \in \Omega$. We must emphasise here that each frequency $\omega_i \in \Omega$, is tried independently from the rest. Then the least-squares spectrum is defined by

$$s(\omega_i) = \frac{\mathbf{f}^T \mathbf{C}_f^{-1} \hat{\mathbf{g}}(\omega_i)}{\mathbf{f}^T \mathbf{C}_f^{-1} \mathbf{f}}, \quad i = 1, 2, \dots, k \quad (5)$$

Equation (5) shows that the least-squares spectrum is a special case of the hindcast skill of a linear regression when the base functions of Φ are trigonometric.

At this point, it is expedient to re-examine Eq. (1) and the partitioning of matrix Φ . Φ_s may include trigono-

metric base functions [Eq. (4)] to describe the periodic components of the series, or others, such as *random walk*, *autoregressive* (AR), *moving average* (MA), and *autoregressive moving average* (ARMA) (Jenkins and Watts 1968; Gelb 1974). When the calculation of the least-squares spectrum is carried out, there will be a simultaneous least-squares solution for the parameters of the process. This, indeed, is a rigorous approach to the problem of hidden periodicities: the parameters of the assumed linear system driven by noise are determined simultaneously with the amplitudes and phases of the periodic components, and with other parameters that describe systematic noise.

We are now in the position to tackle the main subject of this paper, that is, the derivation of probability distribution functions (pdf), which underline the least-squares spectrum for the two distinct cases mentioned in Sect. 1. In the next section, we present all relevant lemmas and theorems needed to derive the probability density functions.

3 Preliminary lemmas and theorems

Before deriving the pdf of the least-squares spectrum \mathbf{s} , it is expedient to refer to a number of useful lemmas and theorems. We consider an m -dimensional stochastic vector \mathbf{X} with its associated covariance matrix \mathbf{C}_x that is, in general, singular. In addition, we assume, without loss of generality, that \mathbf{X} follows the central multidimensional normal distribution. In the following, symbol “ \sim ” means *follows*, “*df*” denotes *degrees of freedom*, “ $\hat{\cdot}$ ” indicates *least-squares estimate*, and “ g^{-1} ” means *g-inverse*.

Lemma 1. Let \mathbf{X} be an m -dimensional stochastic vector from a multidimensional normal distribution $n(\mathbf{0}, \mathbf{C}_x)$, where \mathbf{C}_x may be singular. The random variable $Q = \mathbf{X}^T \mathbf{C}_x^- \mathbf{X}$ is distributed as χ_r^2 where $r = \text{rank } \mathbf{C}_x$ and \mathbf{C}_x^- indicates g -inverse (Rao and Mitra 1971).

Lemma 2. Let \mathbf{X} be an m -dimensional stochastic vector from a multidimensional normal distribution $n(\mathbf{0}, \mathbf{C}_x)$, where \mathbf{C}_x may be singular. Let \mathbf{A} be a symmetric matrix and $r = \text{rank } \mathbf{A}$. The random variable $Q = \mathbf{X}^T \mathbf{A} \mathbf{X}$ is distributed as χ_r^2 , if and only if $(\mathbf{C}_x \mathbf{A})^2 = \mathbf{C}_x \mathbf{A}$, that is, $\mathbf{C}_x \mathbf{A}$ is idempotent (Rao and Mitra 1971, p. 171; Hogg and Craig 1978, p. 413).

Lemma 3. Let Q_1 and Q_2 denote random variables, which are quadratic forms in the items of a random sample \mathbf{X} of size m from a distribution which is $n(\mathbf{0}, \mathbf{C}_x)$. Let \mathbf{A} and \mathbf{B} denote respectively, the real symmetric characteristic matrices of Q_1 and Q_2 . The random variables Q_1 and Q_2 are stochastically independent if and only if $\mathbf{A} \mathbf{C}_x \mathbf{B} = \mathbf{0}$ (Hogg and Craig 1978, p. 414).

Lemma 4. Let Q, Q_1 and Q_2 denote random variables, which are quadratic forms in the items of a random sample \mathbf{X} of size m from a distribution which is $n(\mathbf{0}, \mathbf{C}_x)$. Let Q_1 and Q_2 be stochastically independent and $Q = Q_1 + Q_2$. Then $df(Q) = df(Q_1) + df(Q_2)$ (Hogg and Craig 1978, p. 417).

Theorem 1. Let \mathbf{X} be an m -dimensional stochastic vector from a multidimensional normal distribution $n(\mathbf{0}, \mathbf{C}_x = \sigma_0^2 \mathbf{N}^-)$ where σ_0^2 is a known scale factor (a-priori variance) and \mathbf{N} may be singular of rank r . If the random variable $Q = \mathbf{X}^T \mathbf{C}_x^- \mathbf{X}$ is distributed as the χ_r^2 distribution, then the random variable $\hat{Q} = (1/r) \mathbf{X}^T \hat{\mathbf{C}}_x^- \mathbf{X}$ will be distributed as $F_{r,v}$, where $v = m - u$ are the degrees of freedom used to obtain an estimate for σ_0^2 and $\hat{\mathbf{C}}_x = \hat{\sigma}_0^2 \mathbf{N}^-$.

Proof. We know that $\mathbf{C}_x = \sigma_0^2 \mathbf{N}^-$ and $\hat{\mathbf{C}}_x = \hat{\sigma}_0^2 \mathbf{N}^-$, where \mathbf{N} may be singular. Combining the above two relations, we obtain $\hat{\mathbf{C}}_x^- = \sigma_0^2 / \hat{\sigma}_0^2 \mathbf{C}_x^-$. According to Lemma 1, $\mathbf{X}^T \hat{\mathbf{C}}_x^- \mathbf{X} = \sigma_0^2 / \hat{\sigma}_0^2 \mathbf{X}^T \mathbf{C}_x^- \mathbf{X} \sim \sigma_0^2 / \hat{\sigma}_0^2 \chi_r^2$. But $v \hat{\sigma}_0^2 / \sigma_0^2 \sim \chi_v^2$ and $[\chi_r^2 / r] / [\chi_v^2 / v] \sim F_{r,v}$, thus $(1/r) \mathbf{X}^T \hat{\mathbf{C}}_x^- \mathbf{X} \sim F_{r,v}$.

Theorem 2. Let \mathbf{X} be an m -dimensional stochastic vector from a multidimensional normal distribution $n(\mathbf{0}, \hat{\mathbf{C}}_x = \hat{\sigma}_0^2 \mathbf{N}^-)$, where $\hat{\sigma}_0^2$ is the least-squares estimate of σ_0^2 (a-priori variance) and \mathbf{N} may be singular. Let $\hat{Q} = \mathbf{X}^T \hat{\mathbf{A}} \mathbf{X}$ be a random variable with $\hat{\mathbf{A}} = \hat{\mathbf{C}}_x^- \mathbf{K}$ where \mathbf{K} is an idempotent matrix. If the random variable $Q = \mathbf{X}^T \mathbf{A} \mathbf{X}$, with $\mathbf{A} = \mathbf{C}_x^- \mathbf{K}$ and $\mathbf{X} \sim n(\mathbf{0}, \mathbf{C}_x = \sigma_0^2 \mathbf{N}^-)$ is distributed as the χ_r^2 distribution, then the random variable $\hat{Q} = (1/r) \mathbf{X}^T \hat{\mathbf{A}} \mathbf{X}$ will be distributed as $F_{r,v}$, where $r = \text{rank } \mathbf{A}$ and $v = m - u$ are the degrees of freedom used to obtain the estimate for σ_0^2 .

Proof. We consider an m -dimensional stochastic vector $\mathbf{X} \sim n(\mathbf{0}, \hat{\mathbf{C}}_x)$ and the random variable $\hat{Q} = \mathbf{X}^T \hat{\mathbf{A}} \mathbf{X}$, where $\hat{\mathbf{A}} = \hat{\mathbf{C}}_x^- \mathbf{K}$, and \mathbf{K} is an idempotent matrix. As in the proof of Theorem 1, we can write $\hat{\mathbf{C}}_x = \hat{\sigma}_0^2 / \sigma_0^2 \mathbf{C}_x$, which leads to $\hat{Q} = \mathbf{X}^T \hat{\mathbf{A}} \mathbf{X} = v / (v \hat{\sigma}_0^2 / \sigma_0^2) \mathbf{X}^T \mathbf{A} \mathbf{X}$. Combining Lemma 2 and Theorem 1, we obtain the proof.

4 Least-squares spectrum revisited

So far, we have dealt with the determination of the least-squares spectrum without evaluating the significance of the peaks. This is a very important issue since we need to know which of the peaks are statistically significant and can be suppressed. Expression (5) is not very convenient for the derivation of the pdf of \mathbf{s} . We can write Eq. (2) as

$$\hat{\mathbf{r}} = (\mathbf{I} - \mathbf{J}) \mathbf{f} \quad (6)$$

where \mathbf{I} is the identity matrix and \mathbf{J} is given by

$$\mathbf{J} = \Phi (\Phi^T \mathbf{C}_f^{-1} \Phi)^{-1} \Phi^T \mathbf{C}_f^{-1} \quad (7)$$

Substitution of Eq. (6) into Eq. (5) yields, after some rearrangement

$$\mathbf{s} = \frac{\mathbf{f}^T \mathbf{C}_f^{-1} \mathbf{J} \mathbf{f}}{\mathbf{f}^T \mathbf{C}_f^{-1} \mathbf{f}} \quad (8)$$

Deriving the pdf of the least-squares spectrum as a ratio of two quadratic forms given by Eq. (8) is not an easy task, since the two quadratic forms of the ran-

dom variable \mathbf{f} are not statistically independent, for $\mathbf{C}_f^{-1}\mathbf{J}\mathbf{C}_f\mathbf{C}_f^{-1} \neq \mathbf{0}$ (cf. Lemma 3). However, following Steeves (1981a), we can write the denominator of Eq. (8) as

$$\mathbf{f}^T \mathbf{C}_f^{-1} \mathbf{f} = \mathbf{f}^T \mathbf{C}_f^{-1} \mathbf{J} \mathbf{f} + \mathbf{f}^T \mathbf{C}_f^{-1} (\mathbf{I} - \mathbf{J}) \mathbf{f} \quad (9)$$

Equation (9) shows that the series quadratic form (left-hand side, LHS) has been decomposed into the signal (first term on the right-hand side, RHS) and the noise (second term on the RHS). These two components must now be statistically independent. Indeed, $\mathbf{C}_f^{-1}\mathbf{J}\mathbf{C}_f\mathbf{C}_f^{-1}(\mathbf{I} - \mathbf{J}) = \mathbf{0}$ (cf. Lemma 3), for \mathbf{J} is an idempotent matrix (Mikhail 1976 p. 470). We note here that the independence of the two quadratic forms is retained regardless of the covariance matrix being diagonal or fully populated. Substitution of Eq. (9) into Eq. (8), and rearranging, yields

$$\mathbf{s} = \left[1 + \frac{\mathbf{f}^T \mathbf{C}_f^{-1} (\mathbf{I} - \mathbf{J}) \mathbf{f}}{\mathbf{f}^T \mathbf{C}_f^{-1} \mathbf{J} \mathbf{f}} \right]^{-1} = \left[1 + \frac{Q_n}{Q_s} \right]^{-1} \quad (10)$$

Equation (10) gives the least-squares spectrum as a function of the ratio of two stochastically independent quadratic forms Q_n and Q_s . This ratio is the inverse of the *signal-to-noise* ratio (SNR). It is important to note that Eq. (10) allows us to determine the power spectral density (PSD) of a series from the least-squares spectrum \mathbf{s} (expressed in decibels, dB), by writing the SNR as function of \mathbf{s} , then taking the logarithm and multiplying it by 10 to obtain dB

$$\text{PSD}_{\text{LS}} = 10 \log_{10} \left[\frac{\mathbf{s}}{1 - \mathbf{s}} \right] \quad (11)$$

The PSD given by Eq. (11) is equivalent to the one determined from the FFT method, when the series is equally spaced and equally weighted. Evidently, Eq. (11) can be used to calculate power spectra of any series, without resorting to FFT and its stringent requirements. In addition, Eq. (11) can be used to derive the pdf of the power spectral density and identify significant peaks rigorously. However, this task is beyond the scope of this paper.

At this point we are able to establish the link between the SNR as contained in Eq. (10) and the *canonic hindcast skill* Q_H of a linear regression analysis as defined in Preisendorfer [1988 p. 340, Eq. (9.66)]. As it has been shown in Sect. 2.2, the least-squares spectrum \mathbf{s} is equivalent to the (classic) hindcast skill S_H . Therefore, Eq. (10) can be written as

$$\mathbf{s} = S_H = \frac{1}{1 + \text{SNR}^{-1}} = \frac{\text{SNR}}{1 + \text{SNR}} \quad (12)$$

Comparing Eq. (12) and Eq. (9.68) of Preisendorfer (1988, p. 340) we obtain that the SNR (as defined in this study) is equal to the *canonic hindcast skill* Q_H of the linear regression analysis. The SNR ratio ρ as defined in Preisendorfer [1988, p. 341, Eq. (9.76)] thus differs from ours by a factor equal to the degrees of freedom of the regression analysis.

5 Significance of least-squares spectral peaks

Vaniček, (1971) derived the expected (mean) spectral value of white noise in the least-squares spectrum, assuming that the series consists of statistically independent random values. He pointed out (Vaniček 1971, p. 24) the possibility of deriving magnitudes (threshold values) above which spectral peaks are statistically significant. Lomb (1976), Scargle (1982), Steeves (1981a) and Press and Teukolsky (1988) derived significant levels for the least-squares spectral peaks under the assumption that the series comprises uncorrelated (white) Gaussian noise.

In this paper, we postulate that series \mathbf{f} has been derived from a population of random variables following the multidimensional normal distribution. In the following, we derive the pdf of the least-squares spectrum for the two aforementioned cases regarding the covariance matrix \mathbf{C}_f . It is expedient to note here that the derivation of the pdf is not limited to trigonometric base functions only. Given the similarity of the present development to the regression analysis (Preisendorfer 1988 Sect. 9), the following statistical tests can equally be applied to the linear regression analysis of data series with a fully populated covariance matrix.

5.1 A-priori variance factor σ_0^2 known

Postulating that series \mathbf{f} has been derived from a population of random variables following the multidimensional normal distribution, each of Q_s and Q_n is distributed as the chi-square distribution (χ^2), with μ and ν degrees of freedom, respectively. This is evident from Lemma 2, since $\mathbf{C}_f\mathbf{C}_f^{-1}(\mathbf{I} - \mathbf{J})$ and $\mathbf{C}_f\mathbf{C}_f^{-1}\mathbf{J}$ are both idempotent. As Q_s and Q_n are statistically independent, their ratio is distributed as the *F*-distribution (Hogg and Craig 1978).

Let us suppose that after a number of trials with different base functions we have selected correctly the underlined process of the series, if any, and the form of the systematic noise, both of which have been defined by a set of base vectors of dimension u . We seek the spectral content of the remainder of the series by *successively* fitting base functions of the form of Eq. (4), with frequencies ω_i in the spectral band of interest Ω . The quadratic form of the residual series Q_n will possess $\nu = m - u - 2$ degrees of freedom, where “2” denotes the additional two unknowns for the sine and cosine coefficients of the periodic constituent being forced. It is reminded here that m is the number of data points in the series. Since $Q = Q_s + Q_n = \mathbf{f}^T \mathbf{C}_f^{-1} \mathbf{f}$ and Q_s, Q_n are statistically independent, then $df(Q) = df(Q_s) + df(Q_n) = df(\mathbf{f}^T \mathbf{C}_f^{-1} \mathbf{f}) = m - u$ (Lemma 4). Therefore, $\mu = 2$, $\nu = m - u - 2$. From Lemma 2, $Q_n = \mathbf{f}^T \mathbf{A} \mathbf{f} \sim \chi_\nu^2$, $\nu = m - u - 2$, ($\mathbf{C}_f \mathbf{A}$ is idempotent). Similarly, $Q_s = \mathbf{f}^T \mathbf{B} \mathbf{f} \sim \chi_\mu^2$, $\mu = 2$, ($\mathbf{C}_f \mathbf{B}$ is idempotent). From the above we conclude that $(2/\nu)Q_n/Q_s \sim F_{\nu,2}$.

At this point, it is necessary to recapitulate the null hypothesis H_0 : *The input time series values follow the*

multidimensional normal distribution $n(\mathbf{0}, \mathbf{C}_f)$. H_0 implies that if $Q_n/Q_s \geq (v/2)F_{v,2,\alpha}$, the series will comprise statistically insignificant noise. The alternative hypothesis will be $H_1: Q_n/Q_s < (v/2)F_{v,2,\alpha}$. It makes sense to use only the lower tail end of F , since large values of the ratio Q_n/Q_s (upper tail end of F) imply that the signal is significantly smaller than the noise and therefore is undetectable. Considering Eq. (10), statistically significant spectral peaks will satisfy the following inequality:

$$s(\omega_i) \geq \left[1 + \frac{v}{2}F_{v,2,\alpha}\right]^{-1} \quad (13)$$

It is obvious from Eq. (13) that the least-squares spectrum is distributed as the *beta distribution* (Hogg and Craig 1978 p. 147) with parameters $\gamma = 1$ and $\delta = (m - u - 2)/2$ and, thus, the mean value of the *beta distribution* is $\mu = \gamma/(\gamma + \delta) = 2/(m - u)$. This mean value is the expected spectral value of the noise. We note that this is identical to the mean spectral value of white noise derived by Vaníček (1971) and later by Lomb (1976). Clearly, the assumption of *no correlation* can be relaxed. This shows that the response of the least-squares spectrum is constant (flat) in the frequency domain. In order to make the calculation of the critical value more efficient, without making use of statistical tables, we recall the relation (Rao 1965)

$$F_{v,2,\alpha} = F_{2,v,1-\alpha}^{-1} = \frac{2}{v}(\alpha^{-2/v} - 1)^{-1} \quad (14)$$

Substitution of Eq. (14) into the RHS of Eq. (13) yields the critical value c_α , above which H_0 is rejected and the spectral peaks are significant. The above findings can be summarised in the following theorem.

Theorem 3. Let \mathbf{f} be an m -dimensional stochastic vector from a multi-dimensional normal distribution $n(\mathbf{0}, \mathbf{C}_f)$. Let $\mathbf{C}_f = \sigma_0^2 \mathbf{N}^-$ be the known covariance matrix, where \mathbf{N} may be singular. Let $s(\omega_i)$ represent the least-squares spectrum given by Eq. (10), defined within the spectral band of interest Ω . Let also c_α be a critical value at the significance level α , given by:

$$c_\alpha \left[1 + \frac{1}{\alpha^{-2/v} - 1}\right]^{-1}, \quad v = m - u - 2 \quad (15)$$

where u is the number of unknown parameters estimated by the least-squares procedure.

Then:

- the least-squares spectrum $s(\omega_i)$ follows the beta distribution;
- if $s(\omega_i) \leq c_\alpha \forall \omega_i \in \Omega$ then \mathbf{f} comprises statistically insignificant information (noise) only, at the significance level α within the spectral band of interest,
- if $s(\omega_i) > c_\alpha$, for at least one $\omega_i \in \Omega$, then \mathbf{f} comprises statistically significant component(s) at the significance level α , within Ω ;
- the response of the least-squares spectrum to noise is constant in the frequency domain and its expected spectral value (mean) is $2/(m - u)$.

5.2 A-priori variance factor σ_0^2 unknown – $\hat{\sigma}_0^2$ used

Very often in experimental sciences we obtain time series whose covariance matrix is known up to a scale factor, that is, we use the estimated covariance matrix by scaling the inverse of the matrix of normal equations with the a-posteriori variance factor. When $\hat{\sigma}_0^2$ is an estimate of σ_0^2 and $\mathbf{f} \sim n(\mathbf{0}, \hat{\mathbf{C}}_f = \hat{\sigma}_0^2 \mathbf{N}^-)$, neither quadratic forms Q_s and Q_n will be distributed as the χ^2 distribution, by virtue of $\hat{\sigma}_0^2$ being a random variable. Equation (10) can still be used to evaluate the least-squares spectrum by substituting the inverse covariance matrix with its estimate $\hat{\mathbf{C}}_f^{-1}$. We know that $Q_n \sim \chi_v^2$, and according to Theorem 2, $(1/v)Q_n \sim F_{v,v}$; $\text{rank}[\hat{\mathbf{C}}_f^{-1}(\mathbf{I} - \mathbf{J})] = v = m - u - 2$, since the df used to estimate $\hat{\sigma}_0^2$ are also $v = m - u - 2$. Likewise, since $Q_s \sim \chi_2^2$, then $(1/2)Q_s \sim F_{2,v}$ and Q_n/Q_s will be distributed as the ratio of two F distributions. The derivation of the combined pdf of the ratio of two independent random variables, each distributed as the F distribution, can be found in Appendix 1, according to which, the pdf of $p = \text{SNR}^{-1}$ is given by

$$h_v(p) = \frac{\Gamma(v)\Gamma(\frac{v}{2})}{\Gamma(\frac{v}{2})\Gamma(\frac{v}{2})} p^{(v-2)/2} \int_0^\infty \frac{p^{v/2}}{(1+pq)^v (1+\frac{2}{v}q)^{(v+2)/2}} dq \quad (16)$$

The integral in Eq. (16) is a hypergeometric integral, which can be written in terms of Gauss's hypergeometric function ${}_2F_1$ as (Gradshteyn and Ryzhik 1965 p. 299)

$$h_v(p) = \frac{\Gamma(v)\Gamma(v)}{\Gamma(\frac{v}{2})\Gamma(\frac{3v}{2})} \frac{1}{3p^2} \times {}_2F_1(v/2 + 1, v/2 + 1; 3v/2 + 1; 1 - 2/vp) \quad (17)$$

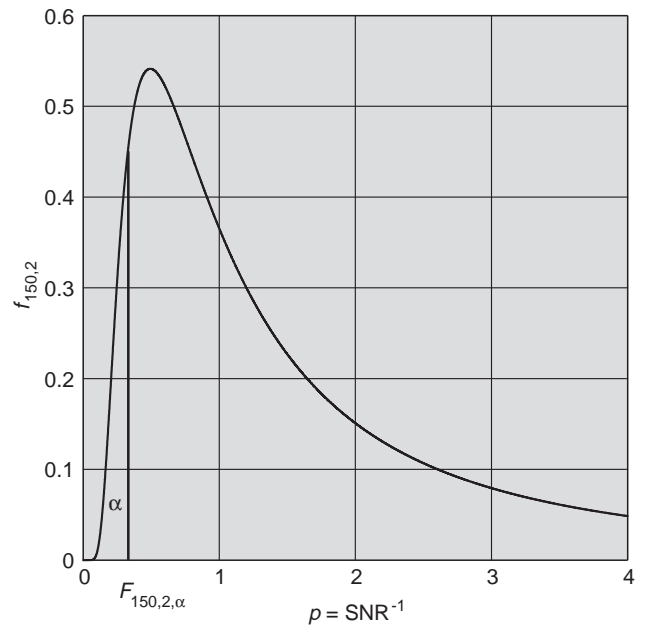


Fig. 1. Plot of $f_{150,2}$ showing the critical value $F_{150,2,\alpha}$ at the significance level α

In Gauss's hypergeometric series ${}_2F_1$, there is a singularity when the time series comprises pure signal only ($p = 0$). Furthermore, in order for the series ${}_2F_1$ to converge, the inequality $|z| = |1 - 2/vp| < 1$ must be satisfied (Luke 1969). As Fig. 2 shows, for small p and v this does not hold true, rendering the series divergent and making Eq. (17) unsuitable for numerical evaluation. However, the hypergeometric integral in Eq. (16) behaves much better numerically, thus Eq. (16) will be used to calculate the probability integral. A plot of $h_v(p)$

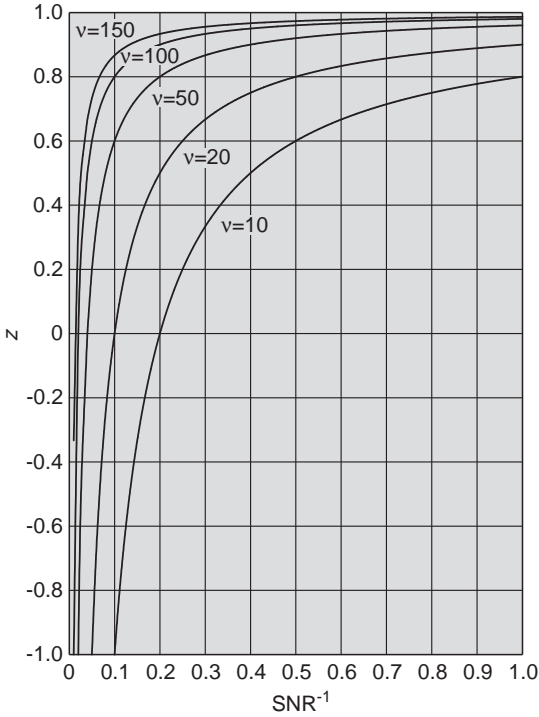


Fig. 2. Variation of z parameter of Gauss's hypergeometric function ${}_2F_1$, as a function of the inverse of the *signal-to-noise* ratio for various degrees of freedom v

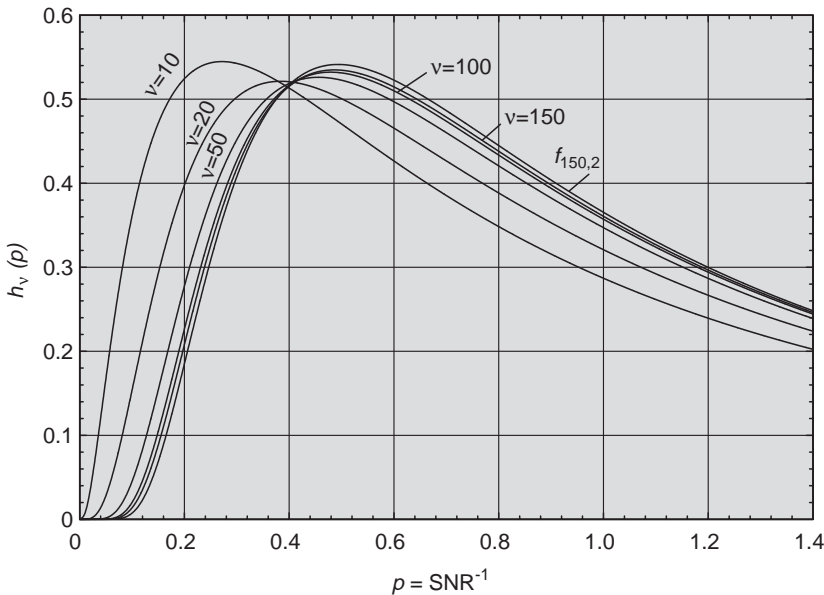


Fig. 3. The probability density function $h_v(p)$ as a function of the inverse of the *signal-to-noise* ratio for various degrees of freedom v . For $v > 150$, $h_v(p)$ converges to $f_{v,2}$

for various degrees of freedom v is shown in Fig. 3. As the degrees of freedom increase (i.e. as the length of the series increases), $h_v(p)$ converges to $F_{v,2}$. This occurs when the series comprises more than about 150 data points and the pdf of the least-squares spectrum converges to the *beta distribution* (as in the first case of known σ_0^2 .)

The probability integral, or cumulative distribution function H_v , can be obtained by numerically integrating equation Eq. (16), the dummy variable being $p = \text{SNR}^{-1}$. Since $h_v(p)$ is the pdf of the inverse SNR, we need to use only the lower tail end of $h_v(p)$. Therefore, the numerical integration can be carried out from zero to a value c_α , such that the integral equals a specified significance level α . Fig. 4 (see also Appendix 2, Table 2) shows the percentage variance level above which spectral peaks are significant at $\alpha = 0.01$, as a function of the degrees of freedom. Similarly, Fig. 5 (see also Appendix 2, Table 3) shows the significant levels at $\alpha = 0.05$. The difference between the two cases, that is, σ_0^2 known or unknown, is significant for short time series of up to about 150 points, and it is more so for decreasing significant levels. It is also pleasing to realise that when we lack exact information about the accuracy of the input series (σ_0^2 unknown) the levels of significance are higher, indicating that we must be stricter in identifying significant peaks. The above are summarised in the following theorem:

Theorem 4. Let \mathbf{f} be an m -dimensional stochastic vector from a multi-dimensional normal distribution $n(\mathbf{0}, \hat{\mathbf{C}}_f)$. Let $\hat{\mathbf{C}}_f = \hat{\sigma}_0^2 \mathbf{N}^{-1}$ be the estimated covariance matrix, where \mathbf{N} may be singular. Let $\mathbf{s}(\omega_i)$ be the least-squares spectrum given by Eq. (10), defined within the spectral band $\mathbf{\Omega}$. Then:

- (a) the inverse of the least-squares SNR follows the hypergeometric probability distribution function given by Eq. (16),

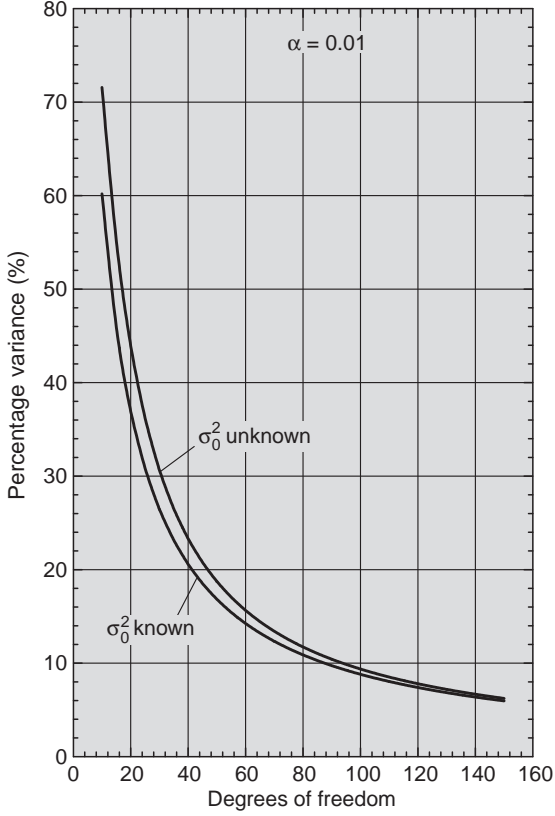


Fig. 4. Critical percentage variance (%) as a function of degrees of freedom at $\alpha = 0.01$

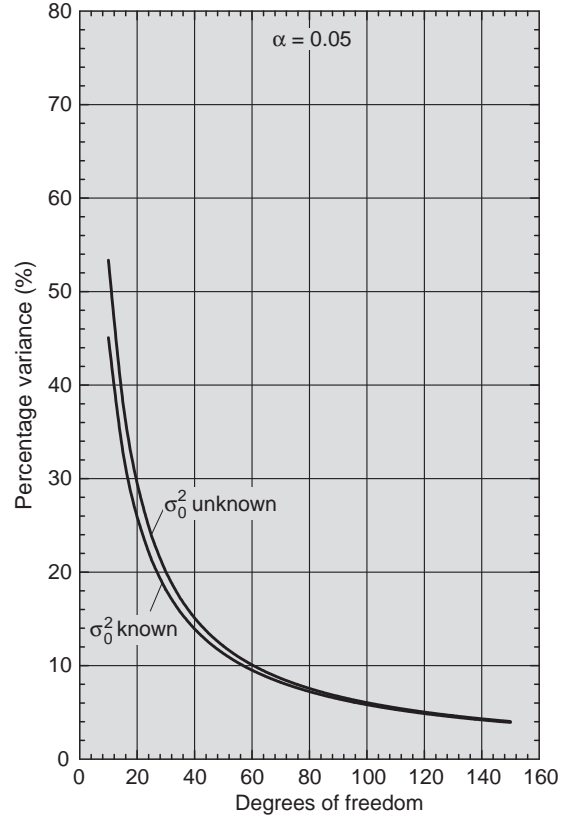


Fig. 5. Critical percentage variance (%) as a function of degrees of freedom at $\alpha = 0.05$

- (b) the critical percentage variance c_α at the significance level α , above which least-squares spectral peaks are statistically significant, is determined by

$$c_\alpha = \left[1 + \frac{v}{2} H_{v,\alpha} \right]^{-1}, \quad v = m - u - 2 \quad (18)$$

where $H_{v,\alpha}$ is the probability integral of $h_v(p)$;

- (c) c_α converges to the critical value determined by Eq. (15), when the series contains more than about 150 data points;
- (d) if $\mathbf{s}(\omega_i) \leq c_\alpha \forall \omega_i \in \Omega$, then \mathbf{f} comprises statistically insignificant information (noise) only, at the significance level α , within Ω ;
- (e) if $\mathbf{s}(\omega_i) > c_\alpha$ for at least one $\omega_i \in \Omega$, then \mathbf{f} comprises statistically significant component(s) at the significance level α , within Ω .

6 Examples

To exemplify the capabilities of the LSSA technique and the usefulness of the statistical tests in the search for significant peaks in the spectrum, we analyse two representative real sample sequences. In the first example, we use the Kay–Marple real sample sequence (Kay and Marple 1981), comprising 64 data points; the LSSA analysis results are compared with the 11 spectral methods summarised in their paper (Kay and Marble pp. 1409–1411). In the second example we make use of the *Westford–Wettzell* baseline length series from very

long baseline interferometry (VLBI) experiments as obtained from the Crustal Dynamics Data Information System (CDDIS 1998) of the National Aeronautics and Space Administration/Goddard Space Flight Center (NASA/GSFC).

6.1 The Kay–Marple example

In this example we make use of the 64-point real sample sequence of Kay and Marple (1981, Table III, p. 1411). The series is equally spaced and equally weighted with no covariance information, thus we choose to perform the statistical testing with an unknown a-priori variance factor at the 99% confidence level, which represents the most stringent option.

In Fig. 6, the top panel shows the series under investigation, panels 1a–4a represent the least-squares spectra of the series corresponding to a four-stage analysis, while panels 1b–4b show the respective least-squares power spectral density (PSD_{LS}) in decibels (dB) [cf. Eq. (11)].

Panel 1a (and 1b) shows the spectrum of the original time series. Clearly, the peaks at frequencies of 0.20 and 0.21 are well resolved and they are both statistically significant. In the second stage of the analysis, we suppress both significant constituents and the spectrum of the residual series is given in panel 2a (and 2b). The peak at frequency of 0.10 is now clearly present, though statistically insignificant. However, the peaks at frequencies

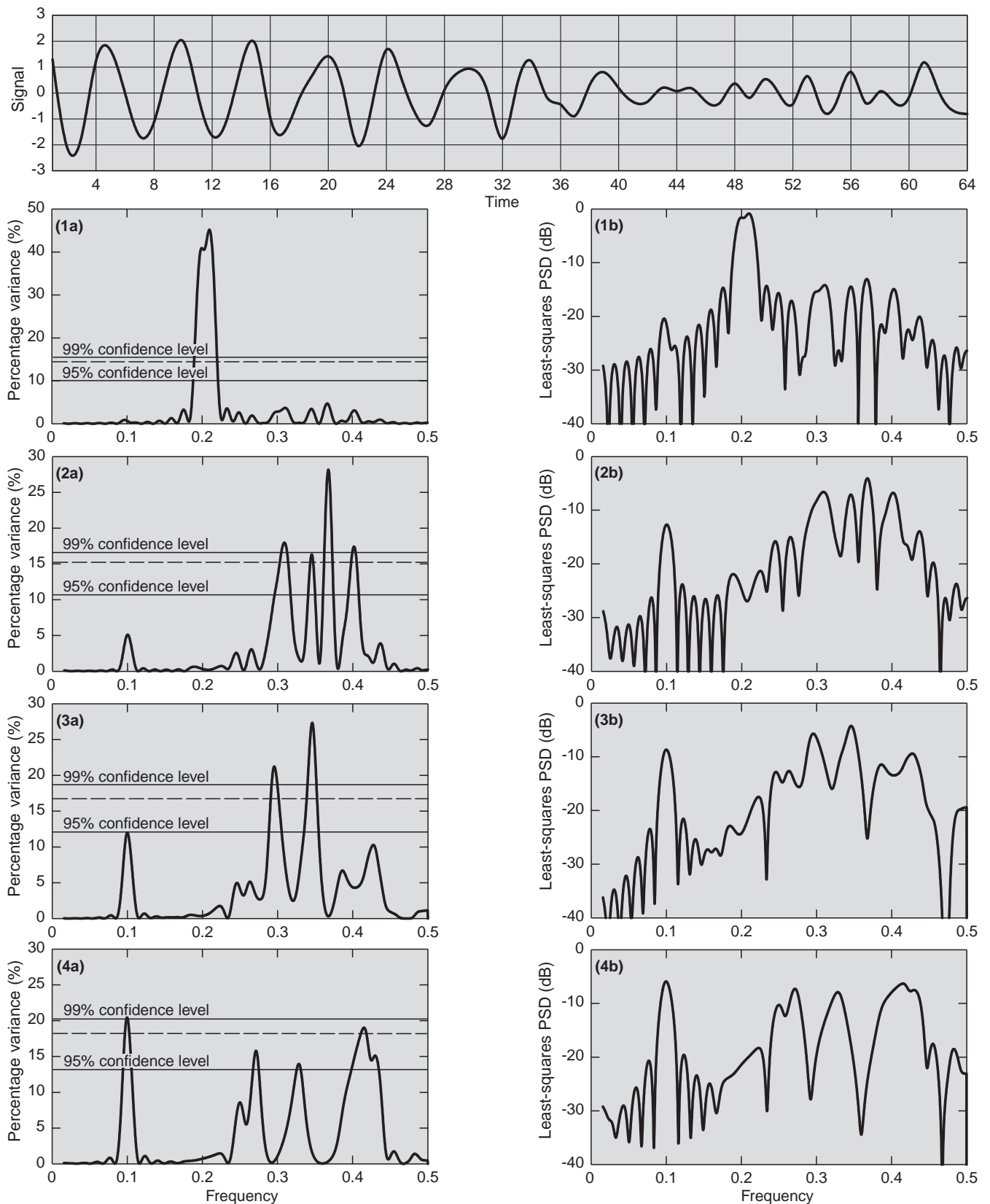


Fig. 6. The Kay–Marple example. The *top panel* shows the real sample sequence. *Panels 1a–4a* show the least-squares spectra and *panels 1b–4b* are the respective least-squares power spectral densities

(PSD) in decibels. The 99% confidence levels correspond to unknown a-priori variance factor (*solid lines*). *Dashed lines* indicate the 99% level for known a-priori variance factor

Table 1. The Kay–Marple real sample sequence analysis using LSSA. Phases are with respect to $t = 1$. The standard errors are formal estimates using the a-posteriori variance factor to scale the inverse matrix of normal equations

No.	Frequency	Amplitude	Phase
1	0.099893	0.0985 ± 0.0286	356.91 ± 1.61
2	0.199581	0.9720 ± 0.0320	356.38 ± 1.79
3	0.209728	0.9836 ± 0.0317	0.41 ± 1.82
4	0.295488	0.1291 ± 0.0286	52.07 ± 1.63
5	0.310720	0.2144 ± 0.0285	155.75 ± 1.64
6	0.346034	0.1506 ± 0.0292	130.71 ± 1.68
7	0.367541	0.2350 ± 0.0293	163.30 ± 1.66
8	0.401515	0.2818 ± 0.0281	121.06 ± 1.65

of 0.311, 0.368 and 0.402 are significant at the 99% confidence level. In a third stage of analysis, the latter three frequencies along with the former two (i.e. 0.20 and 0.21) are suppressed simultaneously and the spectrum of the residual series is given in panel 3a (and 3b). In this residual series, the frequency of 0.10 is at the threshold of the 95% confidence level, while the peaks at 0.295 and 0.346 are significant. In a fourth stage of analysis, the latter two frequencies together with the former five are suppressed simultaneously and the spectrum of the residual series is given in panel 4a (and 4b). It is interesting to note that the frequency of 0.10 is now significant at the 99% confidence level. After suppressing frequency 0.10, the resulting residual series shows a significant peak at 0.415, although of small amplitude (spectrum not shown).

The results of the analysis are summarised in Table 1. Comparison of the first three frequencies and amplitudes (Table 1) with those from Table V of Kay and Marple (1981, p. 1411) reveals that our frequencies (excluding No. 3) and amplitudes are closer to the actual frequencies and amplitudes of the signal (Kay and Marple 1981 p. 1409), although the differences are within the error estimates.

6.2 Westford–Wettzell VLBI baseline

In this example, we use the Westford–Wettzell baseline length series obtained from VLBI experiments. The data were obtained from the Crustal Dynamics Data Information System (CDDIS, 1998) of the NASA/GSFC Internet site. The series comprises 823 unequally-spaced and unequally-weighted observations. We perform the analysis of the series to demonstrate the importance of the variable weights. As the series is sufficiently long, we do not distinguish between known and unknown a-priori variance factors and we choose to work with the 99% confidence level for detecting significant peaks. We emphasise here that we do not intend to search or comment on the causality of the spectral peaks, nor do we strive for a complete analysis of the series, as this is the subject of another investigation.

The top panel in Fig. 7 shows the baseline length variation (millimetres) with the standard error bars. Panels 1a and 1b show the least-squares spectrum and the PSD_{LS} respectively of the original but equally-weighted series. Subsequently, we consider the series

values weighted by the inverse of their variance and the spectrum is shown in panel 2a (and 2b). The threshold value for detecting significant peaks at the 99% confidence level is 1.15%, thus many peaks can be declared as significant. However, we concentrate on the three strongest peaks at periods of 365 days, 181.5 days and 62 days. It is evident from the two spectra (1a and 2a) that the annual peak is much stronger in the weighted spectrum, while the semi-annual and bimonthly peaks are only present in the weighted spectrum. Similar conclusions can be drawn from the analysis of *Richmond–Wettzell* baseline length series (spectra not presented in this paper). The amplitudes of the annual peak for Westford–Wettzell and Richmond–Wettzell series are 4.9 ± 0.4 mm and 3.9 ± 0.4 mm, respectively.

7 Discussion and conclusions

Very often in practice we need to analyse short time series, whose values may be unevenly spaced and weighted, with trends, gaps and datum shifts. Least-squares spectral analysis offers an alternative to FFT techniques in that it can be applied without pre-processing the data. Furthermore, the capability of analysing a series by taking into consideration its associated covariance matrix is of great importance, for we take into account the variable weights and correlation between the values, as well as performing rigorous statistical tests to identify stochastically significant and thus suppressible peaks.

In this paper, we tackled the derivation of the probability density function of the least-squares spectrum for two distinct cases: (a) the covariance matrix of the input series is absolutely known; and (b) the covariance matrix of the input series has an unknown scale defect. The latter case implies that the covariance matrix is unknown and its estimate is used in the determination of the least-squares spectrum. We derived probability density functions for both cases and formulated the criteria of significance of spectral peaks in **Theorems 3 and 4**. We found that the spectral peaks in the case of an unknown covariance matrix must be stronger (higher) than in the case of a known one, in order to be statistically significant. Figures 3 and 4 show that for short series and low significance level values, the distinction between the two cases is important. We must emphasise here that the case of an unknown covariance matrix converges to the case of a known one for series longer than about 150 data points. For example, when the series consists of 150 points, the difference in percentage variance between the two cases is 0.3% at the 99% confidence level and drops to 0.1% when the series comprises 170 points (Tables 2 and 3).

We established the relation between the *least-squares spectrum* and the *power spectral density* in dB [cf. Eq. (11)] and showed the equivalence of the *least-squares spectrum* and the (*classic*) *hindcast skill* of a linear regression analysis [cf. Eq.(12)] as used in the principal component analysis in meteorology and oceanography (e.g. Preisendorfer 1988). Furthermore, we obtained the

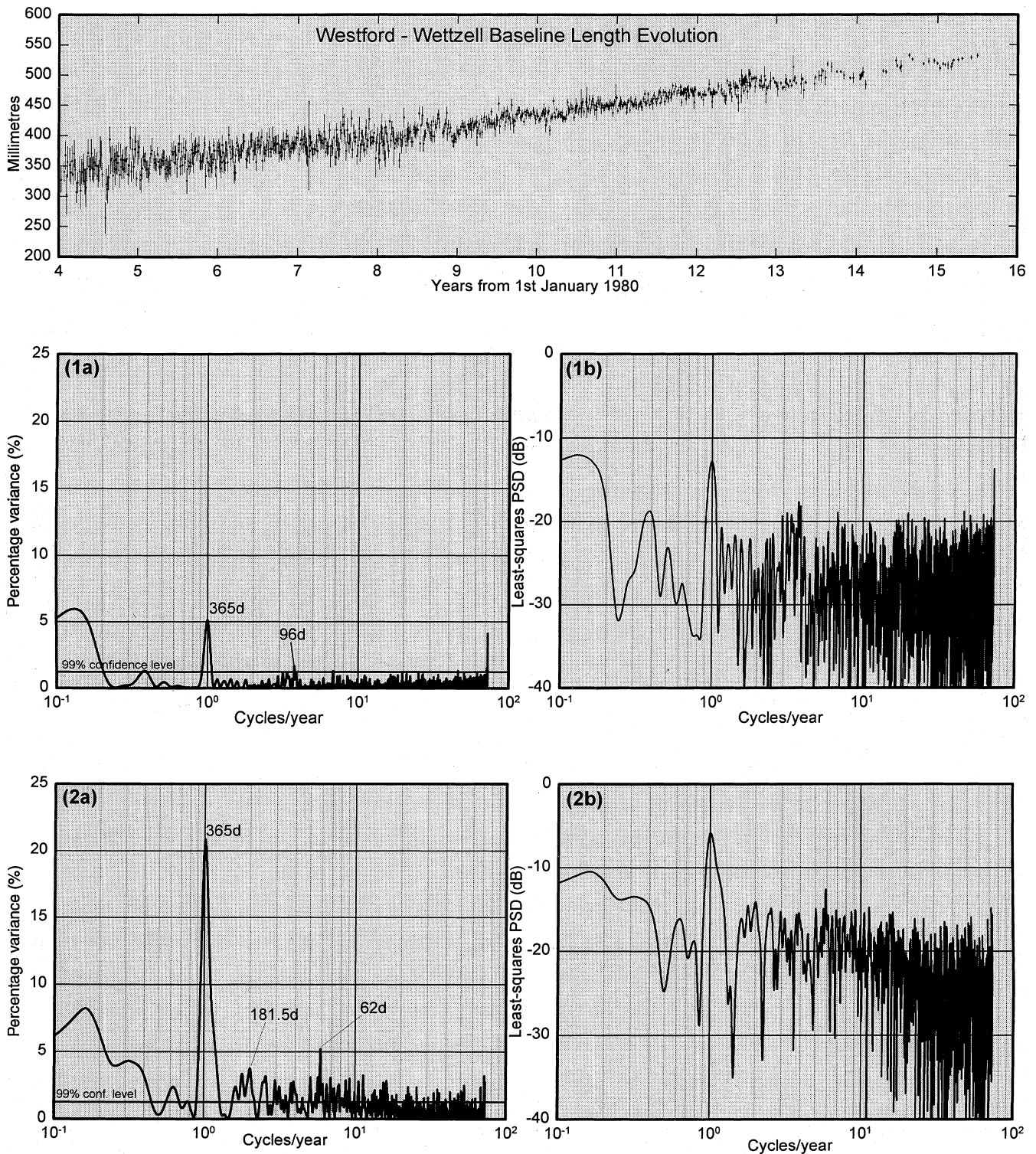


Fig. 7. Westford-Wetzell baseline length analysis. The top panel shows the evolution of the baseline in time. Panels 1a and 1b show the

spectrum of the series when all series values are equally weighted. Panels 2a and 2b show the spectrum of the unequally-weighted series

equivalence of the least-squares *signal-to-noise* ratio and the *canonic hindcast skill* of the linear regression analysis.

We substantiated our findings with two characteristic examples. With the Kay-Marple example we demonstrated the capabilities of the LSSA and the usefulness of

the statistical tests in detecting significant peaks in the spectrum, especially when the series is short. The second example showed the rigour of analysis of unequally spaced and unequally weighted series without pre-processing of the data.

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analysis and the principal component analysis in meteorology and oceanography (hindcast skill of a regression analysis, etc.) was established following the kind recommendation of the late H. van Gysen (2nd reviewer).

Appendix 1

We consider two stochastically independent random variables Q_n and Q_s distributed as $F_{v,v}$ and as $F_{2,v}$, respectively. Here, Q_n represents the quadratic form of the noise and Q_s the quadratic form of the signal. The pdf of the ratio of the above two random variables is derived similarly to the pdf of the ratio of two chi-square variables (e.g. Hogg and Craig 1978, p.145). The F density functions for the random variables Q_n and Q_s are given by

$$f(q_n) = \frac{\Gamma(v)}{\Gamma(\frac{v}{2})\Gamma(\frac{v}{2})} \frac{q_n^{(v-2)/2}}{(1+q_n)^v}, \quad f(q_s) = \frac{1}{(1+\frac{2}{v}q_s)^{(v+2)/2}} \quad (\text{A1})$$

We define a new random variable P

$$P = \frac{Q_n}{Q_s} \quad (\text{A2})$$

Appendix 2

Table 2. Threshold values for various degrees of freedom at the significance level 0.01. Above the threshold values, spectral peaks are statistically significant

Degrees of freedom	σ_0^2 known		σ_0^2 unknown	
	Percentage variance	dB	Percentage variance	dB
10	60.19	1.80	71.57	4.01
15	45.88	-0.72	55.09	0.89
20	36.90	-2.33	43.91	-1.06
25	30.82	-3.51	36.18	-2.47
30	26.44	-4.45	30.63	-3.55
35	23.14	-5.21	26.49	-4.43
40	20.57	-5.87	23.30	-5.18
45	18.51	-6.44	20.77	-5.81
50	16.82	-6.94	18.73	-6.37
55	15.42	-7.39	17.04	-6.87
60	14.23	-7.80	15.63	-7.32
65	13.21	-8.18	14.43	-7.73
70	12.33	-8.52	13.40	-8.10
75	11.56	-8.84	12.51	-8.45
80	10.88	-9.14	11.72	-8.77
85	10.27	-9.41	11.03	-9.07
90	9.73	-9.68	10.41	-9.35
95	9.24	-9.92	9.86	-9.61
100	8.80	-10.16	9.36	-9.86
105	8.40	-10.38	8.91	-10.09
110	8.03	-10.59	8.51	-10.32
115	7.70	-10.79	8.13	-10.53
120	7.39	-10.98	7.79	-10.73
125	7.10	-11.17	7.48	-10.93
130	6.84	-11.34	7.19	-11.11
135	6.60	-11.51	6.92	-11.29
140	6.37	-11.68	6.67	-11.46
145	6.15	-11.83	6.44	-11.62
150	5.96	-11.98	6.22	-11.78

for which we need to find the pdf $h_v(p)$. The following transformation:

$$p = \frac{q_n}{q_s}, \quad q = q_s \quad (\text{A3})$$

maps the set $\mathbf{A} = \{(q_n, q_s); 0 < q_n < \infty, 0 < q_s < \infty\}$ onto the set $\mathbf{B} = \{(p, q); 0 < p < \infty, 0 < q < \infty\}$ and the absolute value of the Jacobian of the transformation is $|\mathbf{J}| = q$. Then, the combined pdf $h(p, q)$ is given by

$$h(p, q) = |\mathbf{J}| f(q_n) \Big|_{q_n=pq} f(q_s) \Big|_{q_s=q} \quad (\text{A4})$$

The marginal distribution $h_v(p)$ will be given by

$$h_v(p) = \frac{\Gamma(v)}{\Gamma(\frac{v}{2})\Gamma(\frac{v}{2})} p^{(v-2)/2} \int_0^\infty \frac{p^{v/2}}{(1+pq)^v (1+\frac{2}{v}q)^{(v+2)/2}} dq \quad (\text{A5})$$

Table 3. Threshold values for various degrees of freedom at the significance level 0.05. Above the threshold values, spectral peaks are statistically significant

Degrees of freedom	σ_0^2 known		σ_0^2 unknown	
	Percentage variance	dB	Percentage variance	dB
10	45.07	-0.86	53.35	0.58
15	32.93	-3.09	38.27	-2.08
20	25.89	-4.57	29.49	-3.79
25	21.31	-5.67	23.88	-5.04
30	18.10	-6.56	20.02	-6.02
35	15.73	-7.29	17.21	-6.82
40	13.91	-7.92	15.08	-7.51
45	12.47	-8.46	13.42	-8.10
50	11.29	-8.95	12.08	-8.62
55	10.32	-9.39	10.99	-9.09
60	9.50	-9.79	10.07	-9.51
65	8.81	-10.15	9.30	-9.89
70	8.20	-10.49	8.63	-10.25
75	7.68	-10.80	8.05	-10.58
80	7.22	-11.09	7.55	-10.88
85	6.81	-11.37	7.10	-11.17
90	6.44	-11.62	6.71	-11.43
95	6.11	-11.86	6.35	-11.69
100	5.82	-12.09	6.03	-11.92
105	5.55	-12.31	5.75	-12.15
110	5.30	-12.52	5.48	-12.37
115	5.08	-12.72	5.24	-12.57
120	4.87	-12.91	5.02	-12.77
125	4.68	-13.09	4.82	-12.95
130	4.50	-13.26	4.64	-13.13
135	4.34	-13.43	4.46	-13.30
140	4.19	-13.59	4.30	-13.47
145	4.05	-13.75	4.16	-13.63
150	3.92	-13.90	4.02	-13.68

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