

# APPLICATION OF THE LEAST-SQUARES SPECTRAL ANALYSIS TO SUPERCONDUCTING GRAVIMETER DATA TREATMENT AND ANALYSIS

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**Abstract:** Data collected from a superconducting gravimeter contain spikes, gaps, datum shifts (offsets) and other disturbances. Data sampling rates are usually higher than required and filtering is the usual procedure that is followed for their decimation. Spikes, gaps and datum shifts are not desirable in the data and often are removed following techniques that are not rigorous and based on intuition. More importantly, the acquired data series are non-stationary by virtue of having variable noise levels; yet, they are assumed stationary when they are cast in a spectral analysis scheme. In this paper a rigorous method is presented for the analysis of the superconducting gravimeter data, based on the parameterisation of unknown quantities in a least-squares scheme, followed by statistical testing and evaluation of the solution. It is shown that there is no need to de-gap and de-spike the data, or pre-process noisy segments due an earthquake. An example is given by analysing a five-day-long series from the Canadian Superconducting Gravimeter Installation (CSGI), in Cantley, underlining the advantages of the approach.

## 1. Introduction

The Global Geodynamics Project (GGP), an international program of observations of temporal variations of the gravity field of the Earth, is co-ordinating the operation of a network of 16 superconducting gravimeters (SG) around the globe, for the purpose of studying a range of important phenomena, such as Earth tides, ocean tide loading, core nutations and core modes. The SGs sample the gravity field every 1-10 s with a precision of one nGal and they are frequently calibrated with absolute gravimeters. The GGP has been scheduled for six years (1997-2003) and data from all stations are being sent to the International Centre of Earth Tides (ICET) in Brussels for further distribution to the scientific community. More details on the GGP can be found in Crossley et al., (1999).

Similar to any other experimental series, the SG data are not continuous due to instrumental failures. Power failures usually introduce short gaps, while the presence of spikes is not unusual. Furthermore, advances in instrument development and our better understanding of the operation of the SG have resulted in improvements in the accuracy of the data and will continue to improve over the life span of the GGP. Precipitation, hydro-geological processes, earthquakes and other disturbances (helium refills, maintenance, calibration, system upgrades) alter significantly the quality and the characteristics of the series, introducing variable noise levels and datum shifts (offsets). Thus, SG time series collected over long periods will be non-stationary by virtue of being unequally weighted.

The majority of the researchers are using almost exclusively fast Fourier transform (FFT) algorithms for the determination of the power spectrum of the SG series. The FFT approach is computationally efficient and produces, in general, reasonable results for a large class of signal processes (Kay and Marple, 1981). However, there are many inherent limitations in the FFT techniques, 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. De-gapping, de-spiking, de-trending and smoothing noisy segments of the data (earthquakes) are part of the routine before an analysis is initiated. Any “data massaging” is subjective, non-rigorous, non-unique and, in general, unsatisfactory.

In order to avoid unnecessary data pre-processing that may corrupt or obliterate the useful information hidden in the series (signal), the Least Squares Spectral Analysis (LSSA) is used in this study as an alternative to the classical Fourier methods. LSSA was first developed by Vaníček (1969; 1971) to bypass all inherent limitations of Fourier techniques, providing 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, 1981, Pagiatakis 1999) and (d) rigorous statistical testing on the significance of spectral peaks can be performed (Pagiatakis, 1999).

In this paper, a brief overview of the LSSA is presented and applied on a segment of the SG series obtained from the Canadian Superconducting Gravimeter Installation (CSGI). The interested reader can find additional details on the LSSA in Pagiatakis (1999).

## 2. Overview of the Least-squares Spectral Analysis

An observed time series can be considered to be composed of *signal*, a quantity of interest, and *noise*, and 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*, that is, it causes the statistical properties of the series to be a function of time.

An observed time series is considered to be represented by  $f(t)$ , where  $f$  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  $C_f$ , that metricises  $f$ .

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

$$g = Mx \quad (1)$$

where  $M=[M_s|M_n]$  is the Vandermonde matrix and  $x^T=[x_s|x_n]^T$  is the vector of unknown parameters. Subscripts  $[s]$  and  $[n]$  refer to the signal and noise, respectively. Matrix  $M$  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  $M$  and  $x$  is arbitrary. We wish to determine the model parameters, such that the difference between  $g$  and  $f$  (residuals) is minimum in the least-squares sense. Using the standard least-squares notation (e.g. Vaníček and Krakiwsky, 1986) we can write:

$$\hat{r} = f - \hat{g} = f - \Phi(\Phi^T C_f^{-1} \Phi)^{-1} \Phi^T C_f^{-1} f. \quad (2)$$

In the above equation,  $\hat{g}$  is the orthogonal projection of  $f$  onto the subspace  $S_d$ , generated by the column vectors of  $M$ . It follows from the *projection theorem* (Oden, 1979) that  $\hat{r} \perp \hat{g}$ . This means that  $f$  has been decomposed into a signal  $\hat{g}$  and noise  $\hat{r}$  (residual series).

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  $\mathbf{f}$ , 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:

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

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

$$\mathbf{M} = [\cos \omega_i t, \sin \omega_i t], \quad i = 1, 2, \dots, k \quad (4)$$

and the orthogonal projection of  $\mathbf{f}$  onto  $\mathbf{S}$  will be different for each  $T_i \hat{\mathbf{W}}$ . We must emphasise here that each frequency  $T_i \hat{\mathbf{W}}$ , is tried independently from the rest. Then the least-squares spectrum is defined by [Pagiatakis, 1999; Eqs. (5) and (10)]

$$s(\omega_i) = \frac{\mathbf{f}^T \mathbf{C}_f^{-1} \hat{\mathbf{g}}(\omega_i)}{\mathbf{f}^T \mathbf{C}_f^{-1} \mathbf{f}} = \left[ 1 + \frac{Q_n}{Q_s} \right]^{-1}, \quad i = 1, 2, \dots, k, \quad (5)$$

where  $Q_n$  and  $Q_s$  are the quadratic forms of the noise and signal respectively.

At this point, it is expedient to re-examine equation (1) and the partitioning of matrix  $\mathbf{M}$ .  $\mathbf{M}_S$  may include trigonometric base functions (Eq. (4)) to describe the periodic components of the series, or other, 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.

Equation (5) gives the least-squares spectrum in percentage variance and it is equivalent to a periodogram, or amplitude spectrum. However, Eq. (5) can be further developed into other forms to provide the researcher with more familiar spectral representations, such as power spectral density (PSD) in decibels (dB) or in units<sup>2</sup>/frequency, where “units” signifies the units

of the time series values. Following Pagiatakis [1999], the least-squares power spectral density in decibels is given by [ibid., Eq. (11)]

$$PSD_{IS} = 10 \log_{10} \left[ \frac{s}{1-s} \right], \quad (\text{dB}). \quad (6)$$

Solving Equation (5) with respect to  $Q_s$  and dividing by the frequency  $f$ , the classical least-squares spectrum can be transformed into a least-squares PSD in units<sup>2</sup>/frequency

$$PSD_{IS} = \frac{Q_n}{f} \left[ \frac{s}{1-s} \right], \quad (\text{units}^2 / \text{frequency}). \quad (7)$$

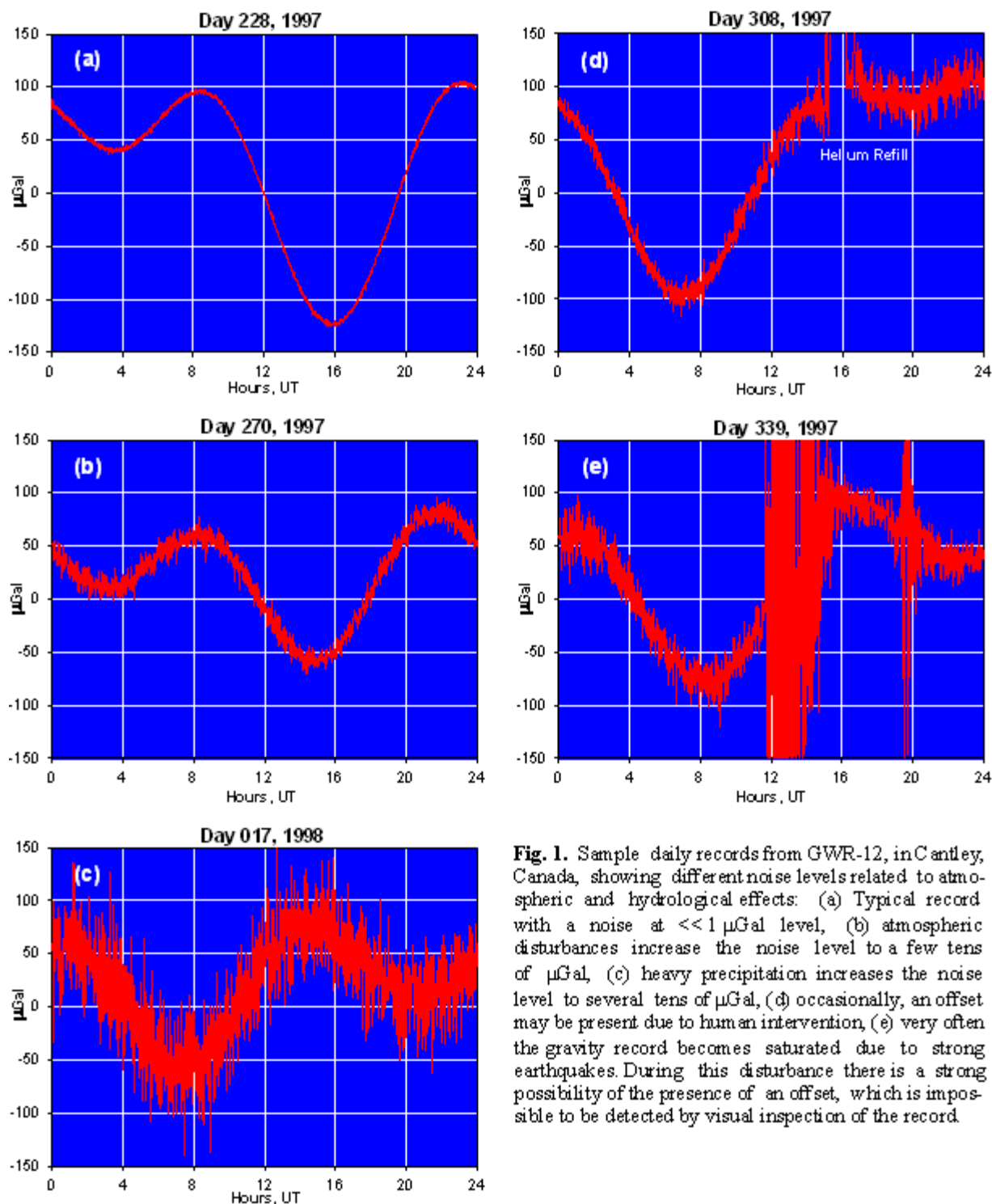
The least-squares *PSD* given by (6) and (7) is equivalent to the one determined from the FFT method, when the series is equally spaced and equally weighted. Evidently, (6) and (7) can be used to calculate power spectra of any series, without resorting to FFT and its stringent requirements.

What follows is a thorough and rigorous analysis of the SG series from the CSGI, using software LSSA v5.0. This software is based on LSSA v1.0 (Wells and Vaní...ek, 1978) and LSSA v2.0 (Wells et. al., 1985). Statistical evaluation of the results of this analysis are based on **Theorem 3** and **Theorem 4** as developed by Pagiatakis (1999) and on other classical statistical tests found in geodetic methodology (e.g. Mikhail, 1976; Vaní...ek and Krakiwsky, 1986).

### 3. CSGI Data Analysis

As it is mentioned in the introduction, similar to any other experimental series, the SG data from the CSGI possess short gaps, spikes, datum shifts (offsets), earthquake disturbances, and atmospheric and hydrological effects. The latter effects introduce increased noise in short time scales, which occasionally can reach many tens of mGal. Figure 1 shows a sample of typical daily records from the Canadian Superconducting Gravimeter Installation (CSGI). On a “quiet” day, the noise level is usually low, reaching an RMS scatter of a few tenths of mGal (Fig. 1a). Atmospheric disturbances, such as heavy precipitation or abrupt change of the atmospheric pressure, increase the noise to several mGal (Fig. 1b), or even to several tens of mGal (Fig. 1c). Human disturbances are also possible, despite the extreme care taken by the personnel when, for instance, transferring liquid helium (Fig. 1d), or repairing certain components of the installation (e.g. cold head replacement). Very often, the record is severely saturated with non-gravity signals, such as those originating from an earthquake (Fig. 1e). Power fluctuations or short interruptions, or sometimes other unknown causes may force the data acquisition system (DAS) to a re-boot. Re-booting of the DAS takes usually a few minutes and this is the cause of short data gaps.

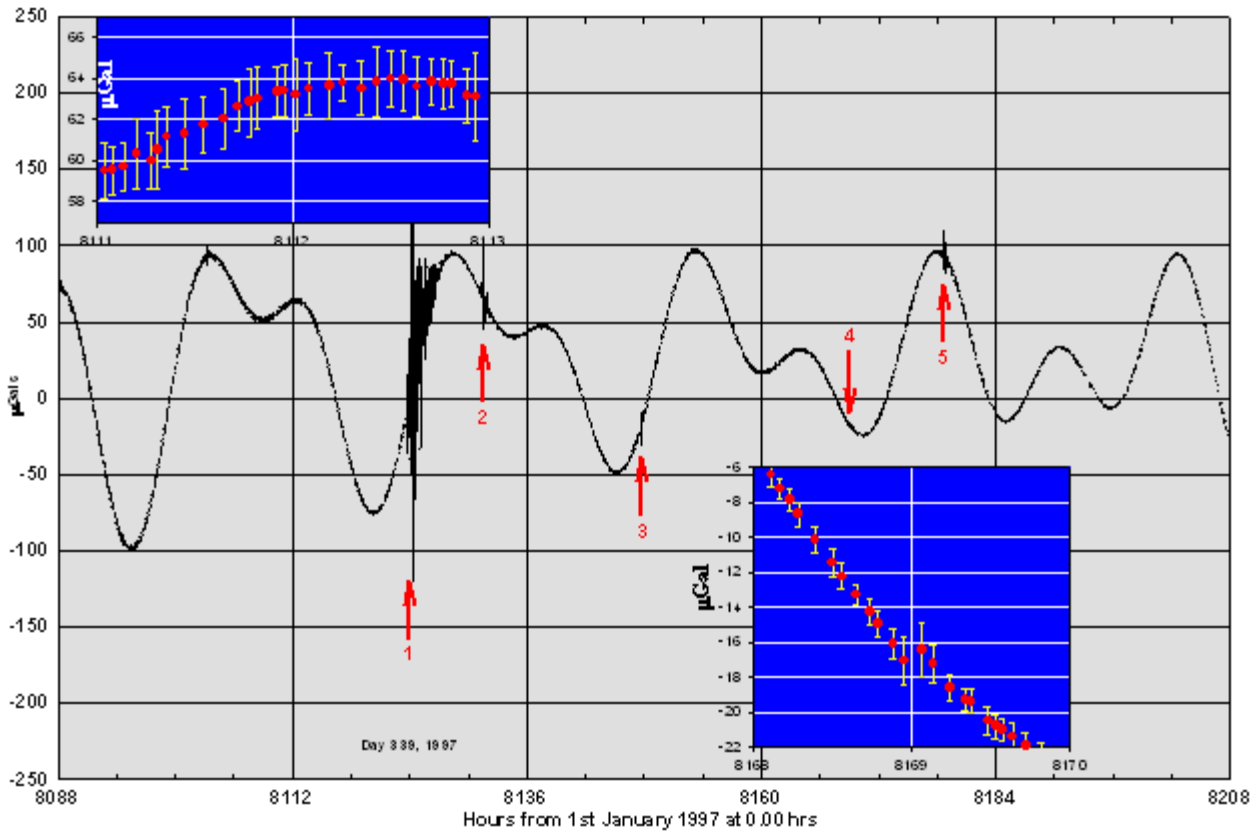
It is our tenet that when such time series are used to detect minute changes of the Earth’s gravity field and in particular those originating from deep interior processes (e.g. core motions), the series have to be treated with great respect! Any pre-processing, such as



**Fig. 1.** Sample daily records from GWR-12, in Cantley, Canada, showing different noise levels related to atmospheric and hydrological effects: (a) Typical record with a noise at  $\ll 1 \mu\text{Gal}$  level, (b) atmospheric disturbances increase the noise level to a few tens of  $\mu\text{Gal}$ , (c) heavy precipitation increases the noise level to several tens of  $\mu\text{Gal}$ , (d) occasionally, an offset may be present due to human intervention, (e) very often the gravity record becomes saturated due to strong earthquakes. During this disturbance there is a strong possibility of the presence of an offset, which is impossible to be detected by visual inspection of the record.

pre-processing. Traditional FFT methods are not offered for such an analysis for the reasons outlined in the introduction.

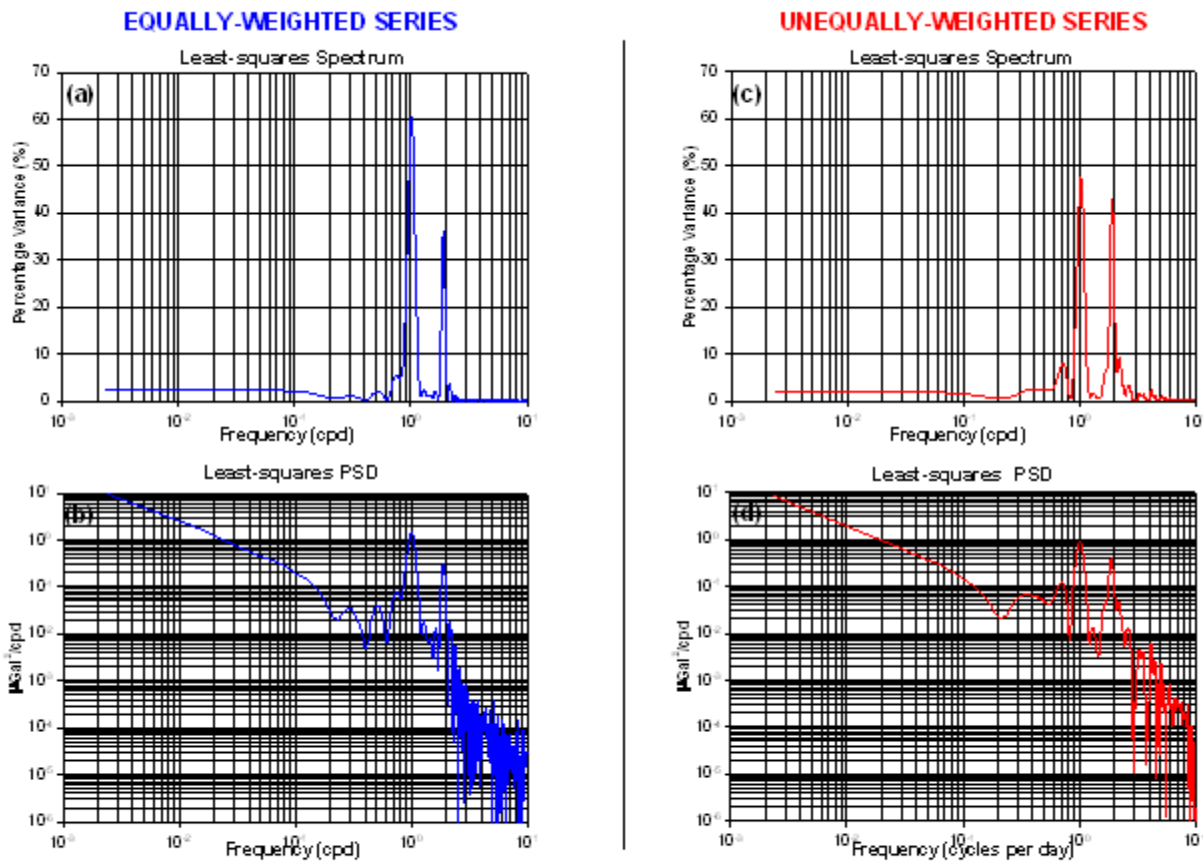
editing, de-gaping, de-spiking, and de-trending, or ignoring the variable noise levels, may obscure or suppress nanogal level signals, yet very important for the studies of the Earth's deep interior. Hence, the series must be analysed as recorded with no



**Fig. 2.** A five-day data segment, produced from the original, 1s data, by applying a Parzen window with  $lag=29s$ . The series is unequally spaced with variances derived from rigorous error propagation of the window variance to the filtered data value. Sampling interval varies at random, between 1-6 minutes. The blue panels show details of the series. Red arrows indicate the location of possible offsets to be considered in the analysis. At  $t=8169$  h (arrow 4) an artificial offset of  $+1\mu Gal$  was introduced.

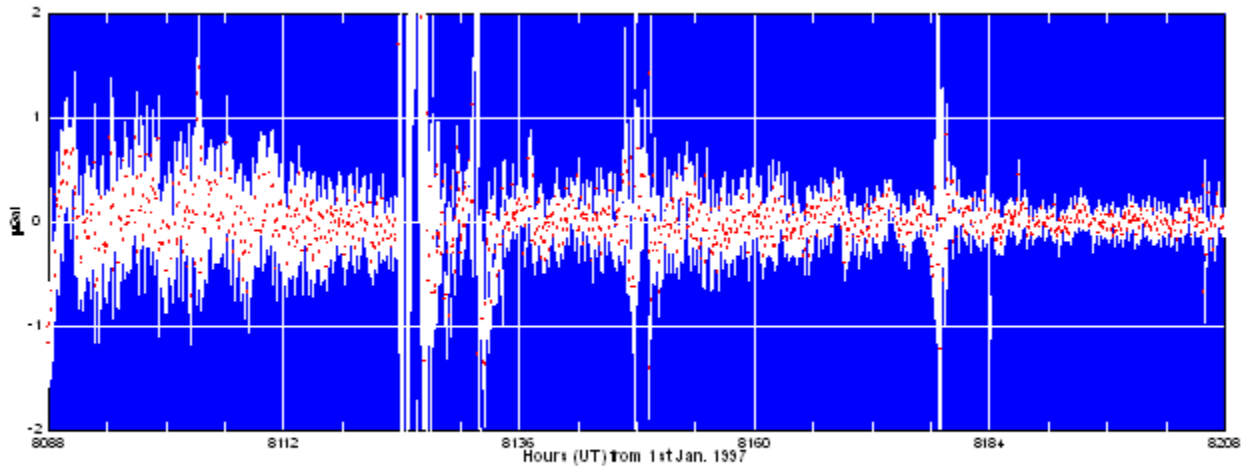
In order to demonstrate our rigorous approach, we select a five-day record from the CSGI, shown in Fig. 2. This record possesses almost all the characteristics usually found in a SG time series. The presence of a nearly two-minute gap renders this segment essentially unequally spaced. Variable noise levels throughout the series require variable weights; simply it is not suitable to assign the same weight to all the series values when their noise level varies significantly (cf. Fig. 1). In addition, the presence of an earthquake (day 339) and other smaller disturbances may have introduced an offset that cannot be detected by a simple visual inspection of the record. Furthermore, we introduce an artificial offset of  $+1$  mGal after  $t=8169$ h (arrow #4) and anticipate that it will be recovered in the analysis. The positions of the other arrows signify the times of possible offsets to be investigated in this analysis.

The original 1s data are filtered in the time domain, using a Parzen window (Jenkins and Watts, 1968) with  $lag=29s$  (total width of 1 minute). This window is used as a weighting function throughout the whole segment, centred at random times with no overlap between successive windows to avoid correlation. Each series value that is included in the window is assumed to have a variance equal to that of the segment being filtered. This variance is propagated through the filtering algorithm to the filtered value. In Fig. 2, the blue panels show details of the series under investigation. Note the variable error bars and the unequal sampling, which in this particular case varies at random between 1-6 minutes. The choice of the Parzen window with  $lag=29s$  is somewhat arbitrary and it is selected here for illustration purposes only. The researcher may experiment with different weighting functions, such as boxcar, triangular, Gaussian, Tukey (e.g. Jenkins and Watts, 1968), or none at all, and with lags other than the one used above. The variable-sampling rate introduced in this analysis eliminates any aliasing arising from the filtering procedure. This is highly desirable in any time series analysis, and the LSSA is the only method that can handle unequally spaced series.



**Fig. 3.** Effect of weighing of time series values in the spectrum. Panels (a) and (b) show the spectrum of the time series in percentage variance (%) and in  $\mu\text{Gal}^2/\text{cpd}$ , respectively, when the series values are equally weighted. Panels (c) and (d) show the spectrum of the time series in percentage variance (%) and in  $\mu\text{Gal}^2/\text{cpd}$ , respectively, when the series values are weighted with the inverse of their variance. Note the difference in the ratios of the diurnal/semi-diurnal peaks.

To illustrate the importance of the proper weighting of the time series values, we produce two spectra for the series. The first spectrum is calculated by choosing equal weights for the series values and it is shown in Fig. 3a, with its respective least-squares PSD ( $\mu\text{Gal}^2/\text{cpd}$ ) in Fig. 3b (cf. Eq. 7). Consequently, assigning variable weights to the series values (inverse of their variance) produces the second spectrum, which is shown in Figures 3c and 3d. It is obvious that the semidiurnal/diurnal peak ratios are different. However, the unequally weighted spectrum reproduces more accurately the theoretical ratios for this location. The interested reader can also refer to Pagiatakis (1999) for a similar example from VLBI series analyses.



**Fig. 4.** Residual series after the suppression of 15 significant constituents (including tidal) and the five (5) offsets indicated by the arrows on Fig. 2. Error bars are 1- $\sigma$  formal errors. Residual series possesses a weighted RMS of 0.18  $\mu\text{Gal}$ .

The next step concerns the analysis of the five-day segment shown in Fig. 2. In this analysis, we are not interested in the tidal constituents; we suppress the tidal waves that are separable within the 5-day span, using their theoretical, well-defined frequencies. We cast the series in a least squares spectral analysis scheme, focusing our attention to the detection and suppression of other significant spectral peaks, as well as to the determination of the five datum shifts indicated by the arrows in Fig. 2. Significant peaks are identified by using **Theorem 3** and **Theorem 4** from Pagiatakis (1999), assuming a 99% confidence level. Following a meticulous identification of spectral peaks, all tidal and non-tidal constituents (15 in total) along with the five offsets are suppressed simultaneously to produce a residual series shown in Fig. 4. The residual series possesses a weighted RMS scatter of 0.18 mGal and the error bars signify 1- $\sigma$  formal errors. Note the increased error bars during the earthquake.

Following the completion of the analysis and evaluation of all the parameters describing the significant constituents of the series, we step back to rerun the analysis without suppressing the five datum shifts. The residual series is shown in Fig. 5 (upper panel). The five arrows indicate, again, the points where offsets may be present. Other than the artificial offset at  $t=8169\text{h}$ , it is nearly impossible to conclude whether the other offsets exist, or even more importantly, whether they are significant or not, just by visually inspecting the series. We will revisit this “identification” issue after we discuss the evaluation of the determined parameters as obtained from the least squares analysis.

In the geodetic methodology of parameter determination using least squares procedures, it is important to evaluate statistically the various steps of the analysis. The application of rigorous, well-established statistical tests can be found in many classical geodetic textbooks (e.g. Mikhail, 1976; Vaní...ek and Krakiwsky, 1986). LSSA software v5.0 is equipped with numerous statistical tests, such as the *goodness-of-fit* test of the residual series, the *chi-square* test of the variance factor, the statistical tests on the significance of peaks in the spectrum ( $F$ , or hypergeometric distribution) and the statistical tests on the significance of the determined parameters ( $F$ , or *chi-square* distribution). We wish to focus here on the statistical evaluation of the vector of determined parameters, including the offsets. It is well known that the vector of determined parameters can be checked for statistical significance with respect to a set of expected or assumed values. These tests are very well documented and applied on a routine basis in



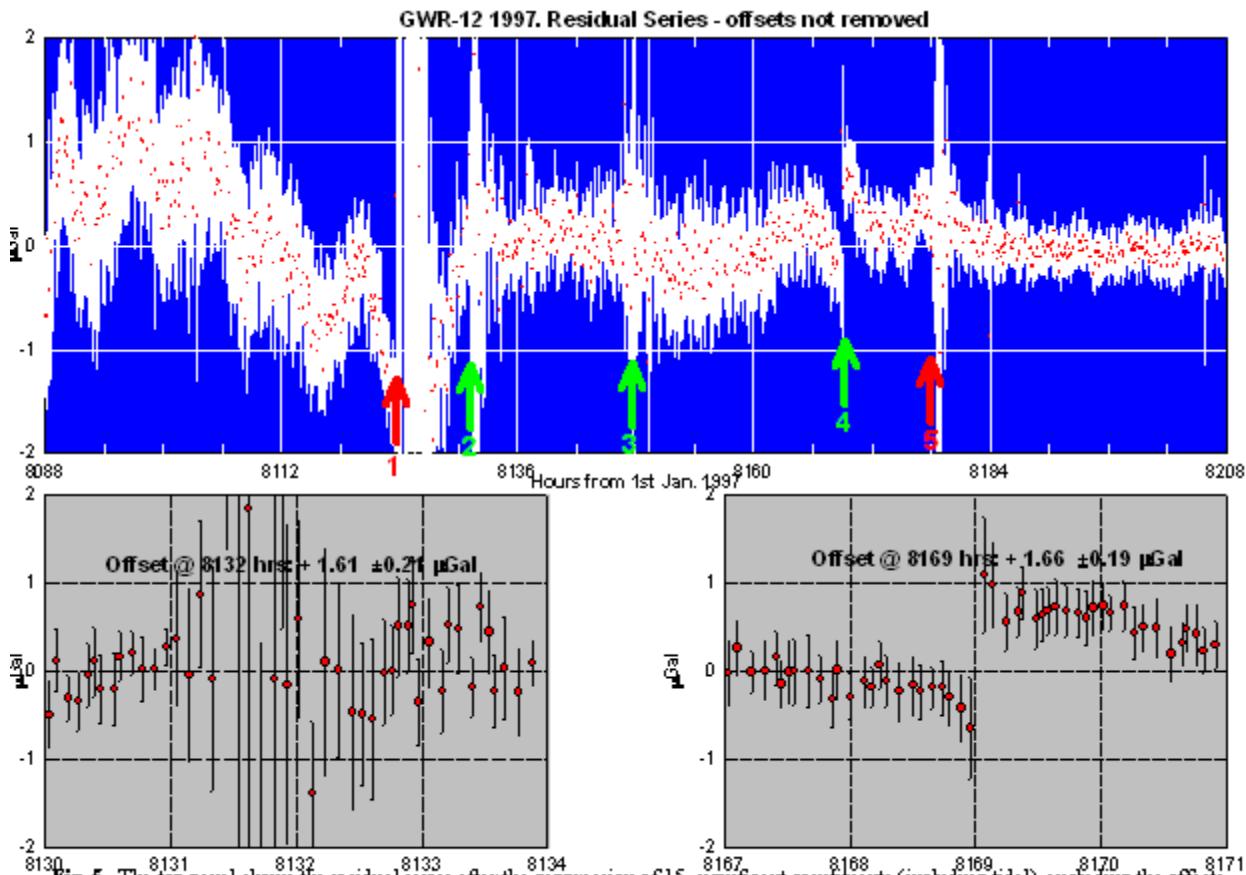


Fig. 5. The top panel shows the residual series after the suppression of 15 significant constituents (including tidal), excluding the offsets indicated by the arrows. Green arrows show offsets that are statistically significant, while red arrows indicate statistically insignificant offsets. The two bottom panels show details of the residual series at two significant offsets (#2 and #4), (see also Table 1).

geodetic problems (e.g. Vaníček and Krakiwsky, 1986, p.239). Often, however, we wish to test the statistical significance of a sub-vector of parameters, or even a single element of it. This is a slightly more involved but well established procedure (e.g. Vaníček and Krakiwsky, 1986; p. 241).

In the case of the present SG data analysis, we test whether the determined offsets are significantly different from zero. This is achieved by comparing the absolute value of each offset separately to its standard error, multiplied by an expansion factor  $C_a$  (see Vaníček and Krakiwsky, 1986; p.241). If the absolute value of the offset is less than the product  $C_a s$ , then the offset will be declared insignificant. The results from the evaluation of all five offsets are summarised in Table 1. In Table 1, column 1 gives the times of the offsets (hours), column 2 is the least-squares estimate of the offsets, whereas their standard error given in column 3. Columns 4 and 5 provide the product of the standard error with the expansion factor  $C_{0.05}=2.89$ , when the *a-priori* variance factor is known, or with  $C_{0.05}=3.04$  when the *a-priori* variance factor is unknown, respectively. Note that the offset at  $t=8149$ hr, is marginally significant. When using a more stringent significance level, i.e.,  $\alpha=0.01$ , then this offset becomes insignificant. In Fig. 5, the green arrows show the times where the offsets are significant, while the red arrows indicate insignificant offsets.

Time (hours)	Offset (mGal)	$s$ (mGal)	$ 2.89s $ (mGal)	$ 3.04s $ (mGal)
8124	+0.41	$\pm 0.22$	+0.64 <i>Insignificant</i>	+0.67 <i>Insignificant</i>
8132	+1.61	$\pm 0.21$	+0.61 <i>Significant</i>	+0.64 <i>Significant</i>
8149	+0.73	$\pm 0.23$	+0.66 <i>Significant</i>	+0.70 <i>Significant</i>
8169	+1.66	$\pm 0.19$	+0.55 <i>Significant</i>	+0.58 <i>Significant</i>
8178	-0.23	$\pm 0.21$	+0.61 <i>Insignificant</i>	+0.64 <i>Insignificant</i>

**Table 1.** Least-squares estimates of the offsets and their standard error (columns 2 and 3). Columns 4 and 5 show the upper limits of the offsets above which they are statistically significant at  $\alpha=0.05$  for known, or unknown *a-priori* variance factor, respectively.

## 5. Discussion and Conclusions

SG time series, like any other experimental series, possess trends, spikes, gaps, atmospheric and earthquake disturbances, as well as variable noise levels. Most importantly, SG series comprise very useful information on various physical processes, such as atmospheric and hydrological phenomena, sea level variations, tides, ocean loading, free oscillations and core motions. Many of these processes are at the nanogal or microgal level (at the most) and they can be easily obscured by the presence of noise in the series. Series editing is dictated by the FFT techniques because all the unwanted disturbances mentioned above simply cannot be handled by this method. Editing may produce artistic and well-composed series but it may, at the same time, obliterate useful information (signal), or even introduce new artificial signals. More importantly, editing is often performed at different non-rigorous pre-analysis stages and the determination of the parameters (e.g. offsets) is merely achieved in a non-simultaneous fashion, that is, the offsets are treated separately from each other and separately from the other parameters.

LSSA can be applied directly to the experimental series without the need of editing or filtering. All unknown parameters are determined simultaneously, whilst rigorous statistical testing is applied to evaluate the residual series and the significance of the determined parameters, either as a vector, or as individual elements. The statistical significance of the peaks is evaluated rigorously (Pagiatakis, 1999) leaving very little room for wrong decisions to be made by the researcher.

The identification and evaluation of offsets in a series is very important. LSSA can evaluate the offsets alongside other parameters. This is achieved by identifying the times at which offsets are suspected and letting the least squares procedure evaluate them. It is imperative to mention here that those offsets, which seem to recover slowly after a few or several hours need not be treated separately from the others. Simply the LSSA solution will show no offset at all, as the best fit of the sinusoid and the other base functions (trends, offsets, etc.) will result in larger residuals in the segment of the offset recovery. In fact, the offset recovery will show perfectly in the residuals.

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