GENERALIZING THE LOMB-SCARGLE PERIODOGRAM

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Abstract. This paper is an elaboration of an issue that arose in the paper "Nonuniform Sampling: Bandwidth and Aliasing" [1]. In that paper the single frequency estimation problem was explored using Bayesian probability theory for quadrature data that were sampled nonuniformly and nonsimultaneously. In the process of discussing single frequency estimation, it was shown that the Lomb-Scargle periodogram is the sufficient statistic for single frequency estimation for a stationary sinusoid given real nonuniformly sampled data. Here we demonstrate that the Lomb-Scargle periodogram may be generalized in a straightforward manner to nonuniformly nonsimultaneously sampled quadrature data when the sinusoid has arbitrary decay. This generalized Lomb-Scargle periodogram is the sufficient statistic for single frequency estimation in a wide class of problems ranging from stationary frequency estimation in real uniformly sampled data, to frequency estimation for a single sinusoid having exponential, Gaussian, or arbitrary decay for either real or quadrature data sampled either uniformly or nonuniformly and for quadrature data nonsimultaneously.

Key words: Nonuniform sampling, Lomb-Scargle periodogram

1. The Lomb-Scargle Periodogram

The Lomb-Scargle periodogram was derived by Lomb [2] using the model

$$d(t_i) = A\cos(2\pi f t_i - \theta) + B\sin(2\pi f t_i - \theta) + n_i \tag{1}$$

where $d(t_i)$ is the data item acquired at time t_i, A and B are the cosine and sine amplitudes of the sinusoid, f is the frequency to be estimated, n_i represents noise at time t_i, and θ was chosen by Lomb to make the sine and cosine model functions orthogonal on the discretely sampled times.

To derive his periodogram, Lomb constrained the amplitudes A and B to their least-squares value. One then obtains,

$$P_{LS}(f) = \frac{R_{LS}(f)^2}{C} + \frac{I_{LS}(f)^2}{S} \tag{2}$$

as the value of Chi-squared (less a constant) where

$$
\begin{aligned}
R_{LS}(f) &\equiv \sum_{i=1}^{N} d(t_i)\cos(2\pi f t_i - \theta), \\
I_{LS}(f) &\equiv \sum_{i=1}^{N} d(t_i)\sin(2\pi f t_i - \theta), \\
C &\equiv \sum_{i=1}^{N} \cos^2(2\pi f t_i - \theta), \\
S &\equiv \sum_{i=1}^{N} \sin^2(2\pi f t_i - \theta)
\end{aligned}
\tag{3}
$$

with θ given by

$$\theta = \frac{1}{2}\tan^{-1}\left(\frac{\sum_{i=1}^{N}\sin[4\pi f t_i]}{\sum_{i=1}^{N}\cos[4\pi f t_i]}\right). \tag{4}$$

This model was later extensively reanalyzed by Jeffrey Scargle [3,4] and, because of the extent of that analysis, this periodogram now bears both Lomb's and Scargle's name.

2. The Generalized Lomb-Scargle Periodogram

As was shown in [1], by applying the rules of Bayesian probability theory to the Lomb model, Eq. (1), this periodogram may be derived in a more theoretically justifiable manner. Knowing this, it is a simple matter to generalize the Lomb model and thus generalize the Lomb-Scargle periodogram to a much wider class of problems. Suppose we have nonuniformly nonsimultaneously sampled quadrature data and we generalize Lomb's model to

$$d_R(t_i) = A\cos(2\pi f t_i - \theta)Z(t_i) + B\sin(2\pi f t_i - \theta)Z(t_i) + n_R(t_i) \tag{5}$$

where $d_R(t_i)$ denotes the real data at time t_i, A and B are the cosine and sine amplitudes, $n_R(t_i)$ denotes the noise at time t_i. Following Lomb's example, θ will be defined in such a way as to make the cosine and sine functions orthogonal on the discretely sampled times. The function $Z(t_i)$ specifies the decay of the sinusoid; $Z(t)$ could be an exponential, a Gaussian, or any other function appropriate to the signal being modeled. If $Z(t)$ is a function of any parameters, those parameters are presumed known; for example, if $Z(t)$ is a decaying exponential, then we are assuming the decay rate constant is known. Of course, in any Bayesian analysis we could turn our attention to the parameters in $Z(f)$ and estimate them, but for this problem we will consider them as known and suppress these parameters from the notation.

In a quadrature data set one also has a measurement of the imaginary part of the signal. The imaginary data are 90° out of phase with the real data. Here this means that model for the imaginary data is 90° out of phase with the model for the real data:

$$d_I(t'_j) = -A\sin(2\pi f t'_j - \theta)Z(t'_j) + B\cos(2\pi f t'_j - \theta)Z(t'_j) + n_I(t'_j) \tag{6}$$

where N_I is the total number of imaginary data values. We have labeled the times with a prime superscript to distinguish them from those in the real data and we have added a subscript, I, to several quantities to indicate that these quantities refer to the imaginary part of the signal.

The posterior probability for the frequency is denoted as $P(f|DI)$, where D stands for all of the data: $D \equiv \{D_R(t_1)\ldots D_R(t_{N_R}), D_I(t'_1)\ldots D_I(t'_{N_I})\}$. In this probability the hypotheses I refers to all of our prior information and does not refer to the imaginary data; rather it refers to the general background information on which this problem is founded. The posterior probability for the frequency is computed from the joint posterior probability for all of the parameters:

$$P(f|DI) = \int dAdBd\sigma P(fAB\sigma|DI) \tag{7}$$

where σ is the standard deviation of the Gaussian noise prior probabilities used to assign the likelihoods. The right-hand side of this equation may be factored using Bayes' theorem and the sum and product rules of probability theory to obtain

$$P(f|DI) \propto \int dAdBd\sigma P(f|I)P(A|I)P(B|I)P(\sigma|I)P(D_R|fAB\sigma I)P(D_I|fAB\sigma I) \tag{8}$$

where we have assumed logical independence of the parameters, and that the standard deviation of the noise prior probability is the same for both the real and imaginary data; i.e., our prior information indicate that real and imaginary data have the same noise levels.

If we assign uniform prior probabilities to $P(f|I)$, $P(A|I)$, $P(B|I)$, a Jeffreys' prior $(1/\sigma)$ to $P(\sigma|I)$, and assign the two likelihoods using Gaussian noise prior probabilities, one obtains:

$$\begin{aligned} P(f|DI) \quad &\propto \quad \int_{-\infty}^{\infty} dA \int_{-\infty}^{\infty} dB \int_0^{\infty} d\sigma \sigma^{-(N+1)} \\ &\times \quad \exp\left\{-\frac{N\overline{d^2} - 2AR(f) - 2BI(f) + A^2C(f) + B^2S(f)}{2\sigma^2}\right\} \end{aligned} \tag{9}$$

where the total data values, N, is defined as

$$N = N_R + N_I. \tag{10}$$

The mean-square data value, $\overline{d^2}$, is defined as

$$\overline{d^2} = \frac{1}{N}\left[\sum_{i=1}^{N_R} d_R(t_i)^2 + \sum_{j=1}^{N_I} d_I(t'_j)^2\right]. \tag{11}$$

The function $R(f)$ is defined as

$$R(f) \equiv \sum_{i=1}^{N_R} d_R(t_i)\cos(2\pi f t_i - \theta)Z(t_i) - \sum_{j=1}^{N_I} d_I(t'_j)\sin(2\pi f t'_j - \theta)Z(t'_j) \qquad (12)$$

which, for uniformly sampled data, reduces to the real part of a weighted discrete Fourier transform of the complex data. The function $Z(t)$ plays the role of the weight or apodizing function. The function $I(f)$ is defined as

$$I(f) \equiv \sum_{i=1}^{N_R} d_R(t_i)\sin(2\pi f t_i - \theta)Z(t_i) + \sum_{j=1}^{N_I} d_I(t'_j)\cos(2\pi f t'_j - \theta)Z(t'_j) \qquad (13)$$

which, for uniformly sampled data, reduces to the imaginary part of the weighted discrete Fourier transform of the complex data. The function $C(f)$ is defined as

$$C(f) \equiv \sum_{i=1}^{N_R} \cos^2(2\pi f t_i - \theta)Z(t_i)^2 + \sum_{j=1}^{N_I} \sin^2(2\pi f t'_j - \theta)Z(t'_j)^2 \qquad (14)$$

and is an effective number of data items in the real part of the measurement, see [1] for more on this. Similarly the function $S(f)$ is defined as

$$S(f) \equiv \sum_{i=1}^{N_R} \sin^2(2\pi f t_i - \theta)Z(t_i)^2 + \sum_{j=1}^{N_I} \cos^2(2\pi f t'_j - \theta)Z(t'_j)^2 \qquad (15)$$

and is the effective number of data items in the imaginary part of the measurement. Finally, the condition that the cross terms cancel, i.e., that the model functions are orthogonal, is used to determine the value of θ. This condition is given by:

$$\begin{aligned} 0 \;=\; & \sum_{i=1}^{N_R} \cos(2\pi f t_i - \theta)\sin(2\pi f t_i - \theta)Z(t_i)^2 \\ - & \sum_{j=1}^{N_I} \sin(2\pi f t'_j - \theta)\cos(2\pi f t'_j - \theta)Z(t'_j)^2. \end{aligned} \qquad (16)$$

Note that if the data are simultaneously sampled, $t_i = t'_i$, Eq. (16) is automatically satisfied, so θ may be defined to be zero. Otherwise, θ is given by

$$\theta = \frac{1}{2}\tan^{-1}\left[\frac{\sum_{i=1}^{N_R}\sin(4\pi f t_i - \theta)Z(t_i)^2 - \sum_{j=1}^{N_I}\sin(4\pi f t'_j - \theta)Z(t'_j)^2}{\sum_{i=1}^{N_R}\cos(4\pi f t_i - \theta)Z(t_i)^2 - \sum_{j=1}^{N_I}\cos(4\pi f t'_j - \theta)Z(t'_j)^2}\right]. \qquad (17)$$

The triple integral in Eq. (9) may be evaluated as follows: First, the integrals over the two amplitudes are uncoupled Gaussian quadrature integrals and are easily done. One needs only complete the square in the exponent, and a simple change of variables to evaluate them. The remaining integral over the standard deviation of the noise prior probability may be transformed into a Gamma integral and is also easily evaluated. We do not give the details of these evaluations; rather we simply give the results:

$$P(f|DI) \propto \frac{1}{\sqrt{C(f)S(f)}} \left[N\overline{d^2} - \overline{h^2}\right]^{\frac{2-N}{2}} \tag{18}$$

where the sufficient statistic $\overline{h^2}$ is given by

$$\overline{h^2} = \frac{R(f)^2}{C(f)} + \frac{I(f)^2}{S(f)} \tag{19}$$

and is a generalization of the Lomb-Scargle periodogram.

3. Discussion

The generalized Lomb-Scargle periodogram, Eq. (19), has a number of very interesting features. First, when the data are real and the sinusoid is stationary, the sufficient statistic for single frequency estimation is the Lomb-Scargle periodogram; not the Schuster periodogram, i.e., not the power spectrum. Second, when the data are real, but $Z(t)$ is not constant, then Eq. (19) generalizes the Lomb-Scargle periodogram in a very straightforward manner to account for the decay of the signal. Third, for uniformly sampled quadrature data when the sinusoid is stationary, Eq. (19) reduces to a Schuster periodogram or the power spectrum of the data. So while the Schuster periodogram is not a sufficient statistic for frequency estimation in real, i.e., nonquadrature, data, it is a sufficient statistic for quadrature data. Fourth, for uniformly sampled quadrature data when the sinusoid is not stationary, Eq. (19) reduced to a weighted power spectrum of the data. Thus the weighted power spectrum is the sufficient statistic for single frequency estimation when the data are quadrature. Fifth, when the quadrature data are nonuniformly but simultaneously sampled, Eq. (19) generalizes the weighted power spectrum to account for the nonuniform samples, but otherwise is the exact analogue of a weighted power spectrum. Finally, when the data are nonuniformly and nonsimultaneously sampled, Eq. (19) generalizes to a functional form that is formally identical to a Lomb-Scargle periodogram but adapted to a decaying sinusoid with quadrature nonuniformly and nonsimultaneously sampled data.

References

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