GENERALIZING THE LOMB-SCARGLE PERIODOGRAM — THE NONSINUSOIDAL CASE

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Abstract. After finishing the paper generalizing the Lomb-Scargle periodogram to the case of quadrature data having a decaying sinusoidal signal [4], I sent a copy of that paper to Jeffrey Scargle thinking that he would enjoy seeing how his periodogram could be generalized. He immediately asked whether or not the periodogram could be generalized to periodic but nonsinusoidal functions. The answer to this is of course yes, but for me it was not a particularly interesting case simply because I work in an NMR lab and in NMR the signals are so nearly sinusoidal that issues concerning nonsinusoidal oscillations never come up. However, in Astrophysics and a host of other applications the issue does come up. So I responded to his email message with a short note that explained how the Lomb-Scargle periodogram could be generalized to the nonsinusoidal but periodic case and then mapped out how those generalizations would go and what the sufficient statistics derived using Bayesian probability theory would be. In this paper, I give a refined version of that calculation and show that the Lomb-Scargle periodogram can be generalized in a way that covers both the sinusoidal and nonsinusoidal cases as well as a host of cases.

Key words: Generalized Lomb-Scargle periodograms, Nonsinusoidal oscillations

1. Introductions

Generalizing the Lomb-Scargle periodogram is not so much an issue of generalizing the periodogram, rather its an issue of generalizing the model used by Lomb to derive the Lomb-Scargle periodogram [1–3]. The Lomb model consists of a single stationary sinusoidal with an extra redundant phase parameter. Lomb choose this phase in such a way as to make the sine and cosine model functions orthogonal on the discretely sampled times. This achieved a tremendous simplification in the way his periodogram appeared and simultaneously made the relationship to the discrete Fourier transform power spectrum obvious. It is the combination of the redundant phase and choosing that phase to make the model orthogonal that defines what I mean by a Lomb type model. In [4] I generalized the Lomb model to a decaying sinusoid that was measured in quadrature. Because of the way the Lomb model was generalized, it subsumed the stationary sinusoidal model used by Lomb as a special case and so that paper showed how the Lomb periodogram generalizes from real data containing a stationary sinusoid, to quadrature data containing arbitrarily decaying sinusoids. Here I would like to generalize the Lomb model to periodic functions in general where the model functions may or may not be sinusoidal.

Suppose we have quadrature data, i.e., a measurement of the real and imaginary parts of a complex signal, and the data has some type of oscillation in it. Here we will assume that the functional form of this oscillation is known, although that is by no means a requirement in a Bayesian calculation. One could easily expand an arbitrary periodic nonsinusoidal signal in a complete set and then proceed with the appropriate Bayesian calculation. This has indeed been done, [5,6]. However, while such a calculation is simple and straightforward, the resulting sufficient statistic are not a "periodogram" in the generally accepted sense of that word. Consequently we will restrict our attention to the case where the model is a known function. The most general model we will consider is of the form

$$\text{Complex Signal} = A e^{Z(f,t) - \mathbf{i} H(f,t)} \tag{1}$$

where A is the intensity of the signal, and the functions $Z(f,t)$ and $H(f,t)$ are otherwise completely arbitrary (except for the presumption that they are periodic functions of frequency f). Of coarse any complex function

$$u(f,t) + \mathbf{i} v(f,t) \tag{2}$$

may be written in this form because

$$u(f,t) + \mathbf{i} v(f,t) = \sqrt{u(f,t)^2 + v(f,t)^2} \exp\left\{ \mathbf{i} \tan^{-1}\left[\frac{v(f,t)}{u(f,t)}\right]\right\}. \tag{3}$$

The functions $Z(f,t)$ and $H(f,t)$ can be identified explicitly if we multiple by the amplitude A, and place the square root in the exponent:

$$A[u(f,t) + \mathbf{i} v(f,t)] = A \exp\left\{ \log\sqrt{u(f,t)^2 + v(f,t)^2} + \mathbf{i} \tan^{-1}\left[\frac{v(f,t)}{u(f,t)}\right]\right\}. \tag{4}$$

Inspecting this equation we find

$$H(f,t) = -\tan^{-1}\left[\frac{u(f,t)}{v(f,t)}\right] \quad \text{and} \quad Z(f,t) = \log\sqrt{u(f,t)^2 + v(f,t)^2}. \tag{5}$$

Consequently any arbitrary periodic complex function may be used as a model in this calculation.

Implicit in this calculation and in the Lomb-Scargle periodogram, is the assumption that the model is a single frequency model. Consequently, when we compute the joint posterior probability for the frequency it is only applicable to data that are known to contain a single resonance. If the data contain multiple resonances, Bayesian probability leads to a simple procedure for estimating multiple frequencies, its just that the statistics that come out of these calculations are not generalizations of the Lomb-Scargle periodogram.

The model, Eq. (1), is not yet sufficient to model a complex data set nor is it in the form that will yield a generalized Lomb-Scargle type periodogram. To model a complex signal, we must insert a phase parameter ϕ into this model. This phase parameter simply tells us where in a cycle the start of data acquisition occurred, one obtains

$$\text{Complex Signal} = A\mathrm{e}^{Z(f,t)-\mathrm{i}H(f,t)-\mathrm{i}\phi}. \tag{6}$$

To make this model a generalized Lomb-Scargle model, we must also add a redundant phase θ:

$$\text{Complex Signal} = A\mathrm{e}^{Z(f,t)-\mathrm{i}H(f,t)-\mathrm{i}\phi-\mathrm{i}\theta}. \tag{7}$$

For now we will assume θ know, and derive its functional dependence on $Z(f,t)$ and $H(f,t)$ later.

If we now separate this equation into its real and imaginary parts and use it to model the quadrature data, one obtains:

$$d_R(t_i) = a\cos[H(f,t_i)-\theta]\mathrm{e}^{Z(f,t_i)} + b\sin[H(f,t_i)-\theta]\mathrm{e}^{Z(f,t_i)} + \text{error} \tag{8}$$

for the real data, where "error" represents the misfit between the data and the model; $d_R(t_i)$ denotes a real data item acquired at time t_i. Similarly for the imaginary data one obtains

$$d_I(t'_j) = b\cos[H(f,t'_j)-\theta]\mathrm{e}^{Z(f,t'_j)} - a\sin[H(f,t'_j)-\theta]\mathrm{e}^{Z(f,t'_j)} + \text{error}. \tag{9}$$

We have made a change of variables, $a = A\cos(\phi)$ and $b = -A\sin(\phi)$, to switch form polar coordinates (A,ϕ), to Cartesian coordinates (a,b), and we have denoted the acquisition time of the imaginary or quadrature data as t'_j to indicate that the times at which the quadrature data were acquired may be different from the times at which the real data were acquired.

2. The Generalized Lomb-Scargle Periodogram

To generalize the Lomb-Scargle periodogram we now apply the rules of Bayesian probability theory using the generalized Lomb model, Eq. (7), and derive the marginal posterior probability for the frequency f independent of the two amplitudes a and b and independent of the standard deviation of the noise prior probability σ. This marginal probability density function is denoted as $P(f|DI)$ where this should be read as the marginal posterior probability for the frequency given all of the data $D \equiv \{D_R, D_I\}$ and the background information I. This background information includes the quadrature nature of the signal as well as the assumption that the model is known. We have denoted the real and quadrature data as $D_R \equiv \{d_R(t_1),\ldots,d_R(t_{N_R})\}$ and $D_I \equiv \{d_I(t'_1,\ldots,d_I(t'_{N_I})\}$ respectively. The number of data items in the real and quadrature data sets have been denoted as N_R and N_I.

The marginal posterior probability for the frequency is computed from the joint posterior probability for all of the parameters appearing in the model:

$$P(f|DI) = \int dadbd\sigma P(fab\sigma|DI) \tag{10}$$

where the integrals result from the application of the sum rule of probability theory. Assuming logical independence, one can factor the right-hand side of this equation to obtain

$$P(f|DI) \propto \int dadbd\sigma P(f|I)P(a|I)P(b|I)P(\sigma|I)P(D_R|fab\sigma I)P(D_I|fab\sigma I) \tag{11}$$

where we have dropped a normalization constant. Assigning uniform prior probabilities to $P(f|I)$, $P(a|I)$ and $P(b|I)$, a Jeffreys' prior to $P(\sigma|I)$ and Gaussians to noise prior probabilities, one obtains

$$\begin{aligned} P(f|DI) \quad &\propto \quad \int_{-\infty}^{\infty} da \int_{-\infty}^{\infty} db \int_0^{\infty} d\sigma \sigma^{-(N+1)} \\ &\times \quad \exp\left\{-\frac{N\overline{d^2} - 2aR(f) - 2bI(f) + a^2C(f) + b^2S(f)}{2\sigma^2}\right\} \end{aligned} \tag{12}$$

where the quantities appearing in this equation are defined in a way analogous to those given in [4]. The total number of data values, N, is defined as

$$N = N_R + N_I. \tag{13}$$

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

$$\overline{d^2} = \frac{1}{N}\left[\sum_{i=1}^{N_R} d_R(t_i)^2 + \sum_{j=1}^{N_I} d_I(t'_j)^2\right]. \tag{14}$$

The function $R(f)$ is defined as

$$\begin{aligned} R(f) \quad &\equiv \quad \sum_{i=1}^{N_R} d_R(t_i)\cos[H(f,t_i) - \theta]\mathrm{e}^{Z(f,t_i)} \\ &- \quad \sum_{j=1}^{N_I} d_I(t'_j)\sin[H(f,t'_j) - \theta]\mathrm{e}^{Z(f,t'_j)}. \end{aligned} \tag{15}$$

Similarly, $I(f)$ is defined as

$$\begin{aligned} I(f) \quad &\equiv \quad \sum_{i=1}^{N_R} d_R(t_i)\sin[H(f,t_i) - \theta]\mathrm{e}^{Z(f,t_i)} \\ &+ \quad \sum_{j=1}^{N_I} d_I(t'_j)\cos[H(f,t'_j) - \theta]\mathrm{e}^{Z(f,t'_j)}. \end{aligned} \tag{16}$$

The function $C(f)$ is defined as

$$C(f) = \sum_{i=1}^{N_R} \cos^2[H(f,t_i) - \theta] e^{2Z(f,t_i)} + \sum_{j=1}^{N_I} \sin^2[H(f,t'_j) - \theta] e^{2Z(f,t'_j)} \tag{17}$$

and is an effective number of data items in the real channel. Similarly, the function $S(f)$ is defined as

$$S(f) = \sum_{i=1}^{N_R} \sin^2[H(f,t_i) - \theta] e^{2Z(f,t_i)} + \sum_{j=1}^{N_I} \cos^2[H(f,t'_j) - \theta] e^{2Z(f,t'_j)} \tag{18}$$

and is an effective number of data values in the imaginary channel. Finally, the condition that the model be orthogonal, i.e., that the quadratic term involving ab be zero in Eq. (12), is

$$\begin{aligned} 0 &= \sum_{i=1}^{N_R} \cos[H(f,t_i) - \theta] \sin[H(f,t_i) - \theta] e^{2Z(f,t_i)} \\ &- \sum_{j=1}^{N_I} \sin[H(f,t'_j) - \theta] \cos[H(f,t'_j) - \theta] e^{2Z(f,t'_j)}. \end{aligned} \tag{19}$$

For simultaneous sampling, this condition is automatically satisfied and we defined θ to be zero; otherwise θ is given by

$$\theta = \frac{1}{2} \tan^{-1} \left(\frac{\sum_{i=1}^{N_R} \sin[2H(f,t_i)] e^{2Z(f,t_i)} - \sum_{j=1}^{N_I} \sin[2H(f,t'_j)] e^{2Z(f,t'_j)}}{\sum_{i=1}^{N_R} \cos[2H(f,t_i)] e^{2Z(f,t_i)} - \sum_{j=1}^{N_I} \cos[2H(f,t'_j)] e^{2Z(f,t'_j)}} \right). \tag{20}$$

The triple integral in Eq. (12) may be evaluated as follows: First, the integral over the two amplitudes are uncoupled Gaussian quadrature integrals and are easily evaluated. 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:

$$P(f|DI) \propto \frac{1}{\sqrt{C(f)S(f)}} \left[N\overline{d^2} - \overline{h^2} \right]^{\frac{2-N}{2}} \tag{21}$$

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

$$\overline{h^2} = \frac{R(f)^2}{C(f)} + \frac{I(f)^2}{S(f)} \tag{22}$$

and is a generalization of the Lomb-Scargle periodogram that includes both the nonsinusoidal and sinusoidal cases, as well as a host of others special cases depending on the functions $Z(f,t)$ and $H(f,t)$.

3. Discussion

To see that this sufficient statistic subsumes the Lomb-Scargle periodogram as a special case all one needs to do is to substitute

$$H(f,t) = 2\pi f t \quad \text{and} \quad Z(f,t) = 0 \tag{23}$$

and, because the Lomb model assumes real data, $N_I = 0$; one obtains

$$\overline{h^2} = \frac{\left(\sum_{i=1}^{N_R} d_R(t_i)\cos[2\pi f t_i - \theta]\right)^2}{\sum_{i=1}^{N_R}\cos^2[2\pi t_i - \theta]} + \frac{\left(\sum_{i=1}^{N_R} d_R(t_i)\sin[2\pi f t_i - \theta]\right)^2}{\sum_{i=1}^{N_R}\sin^2[2\pi t_i - \theta]} \tag{24}$$

which is the Lomb-Scargle periodogram. Additionally, it is easy to show that if $\exp\{Z(f,t)\} \to Z(f,t)$, and $N_I \neq 0$ this statistic reduces to what was found for decaying sinusoids in [4].

The generalized Lomb-Scargle periodogram, Eq. (22), reduced to the Lomb-Scargle periodogram for a real stationary sinusoid. It generalizes the Lomb-Scargle periodogram to the case of a real decaying sinusoid for either uniformly or nonuniformly sampled data. It then generalizes to the Schuster periodogram for a stationary sinusoid when the data are quadrature. It generalizes to a weighted power spectrum when the sinusoid decays for simultaneously sampled quadrature data; the weight function being the decay envelope of the sinusoid. When the data are not simultaneously sampled, the statistic generalizes again to a Lomb-Scargle type periodogram. Finally, Eq. (22) generalizes the Lomb-Scargle periodogram to single frequency estimation when the signal is periodic but not sinusoidal.

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