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Comparing significance criteria for cyclic modulations in time series

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ABSTRACT

General solutions are derived for least-squares fits of amplitude, phase shift and baseline shift of sinusoidal modulations to normally distributed time series. Four cases are compared: weighted and unweighted fit, with and without a baseline shift. Computer simulations have been performed of the statistical distribution of the amplitude resulting from fits to white noise. A normalised amplitude is defined which follows exactly a Rayleigh distribution, even for small, uneven-sampled data sets. Equations are provided for the width of the distribution and the cumulative probability function. A simple criterion for the statistical significance of the amplitude fitted to a time series is derived and compared for equivalence with the Lomb–Scargle criterion based on a power function.

1. Introduction

There is a vast literature on the statistical probability of finding cyclic modulations in noise-generated time series, involving various mathematical techniques, such as Fourier analysis, maximum likelihood and least-squares methods, or a Bayesian approach [1–20]. Fields of application are quite diverse, including e.g. astrophysical observations [3,16,17], the distribution of wind speed [18], height of sea waves [19], and sound reverberation in rooms [20]. Ref. [1] provides additional references pertaining to applications in vibration monitoring, speech analysis, meteorology, economics, radar and sonar technology, seismology, medical diagnostics, etc. In radionuclide metrology, the search for cyclic modulations is a topic in the debate on possible violations of the exponential-decay law [21–30], which is the foundation of the measurement system and nuclear dating [31–37]. At the core of the problem is the need for rigorous and complete uncertainty assessments [38–45] to estimate the magnitude of cyclic effects that can be expected from random and systematic variations in activity measurements repeated over a long period.

The Lomb–Scargle (L–S) periodogram [2–17] is a convenient tool to investigate periodicity of unequally spaced data, as it stems from Fourier analysis, but coincides with the solutions provided by other approaches. Whereas the L–S periodogram was defined for the most simple case of an unweighted fit of a sinusoidal modulation [5,7], equations have been presented to take into account an additional baseline parameter, symmetric and asymmetric weighting of the data, and a moving time window [2,3,6,10,13,15]. The result is a power spectrum over a frequency range, in which the height of local peaks indicate the frequencies at which the modulations in the data set may be statistically significant. The standard formula for the probability of obtaining a peak of power S or more from normally distributed random fluctuations is $P = e^{-S}$.

The periodogram is equivalent to a least-squares method applying sine fit functions with amplitude A and phase shift φ. Pommé and De Hauwere [14] performed computer simulations of least-squares fits of sinusoidal functions to normally distributed white noise. They demonstrated that the fitted amplitudes can be normalised to a value A' which follows a Rayleigh probability distribution, even for small data sets. The width of the distribution is proportional to a standard deviation $\sigma_{A'}$, and the probability that the amplitude A' exceeds k times $\sigma_{A'}$ is $P = e^{-k^2/2}$. In this work, the significance criterion – which reflects the probability for finding an amplitude equal or larger than the fit result – is compared to the criterion derived from the power of the L–S periodogram.

2. Weighted LSQ fit ($C \neq 0$)

2.1. Sinusoidal fit to time series

A time series $y(t)$ of n data pairs is considered in which y_i ($i = 1, \ldots, n$) is random noise drawn from normal distributions $\mathcal{N}(0, \sigma_i^2)$ and t_i is a time variable randomly selected over an interval which covers at least one full period of a sine wave with angular frequency $\omega = 2\pi f$. A trial sinusoidal function is fitted to the data set

$$y(t) = A \sin(\omega t + \varphi) + C \tag{2.1}$$

– adjusting the free parameters of the amplitude A, the phase shift φ, and a baseline shift C – to minimise the square deviations between

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measurements and model, relative to the variances of the y data

$$\chi^2 = \sum_{i=1}^{n} \left(\frac{y_i - y(t)}{\sigma_i} \right)^2 \tag{2.2}$$

Eq. (2.1) represents a case of linear regression of y as a function of x,

$$x = \sin(\omega t + \varphi) \tag{2.3}$$

in which x follows an Arcsine distribution in the interval [a, b] = $[-1, 1]$. For a sufficiently large, random data set, the variance of x will converge to its expectation value $(b-a)^2/8 = 1/2$ [14]. Equations for A, C and φ can be derived from the condition that the LSQ solution corresponds to a minimum in χ^2 (Eq. (2.2)). In the remainder of the text, the summation signs pertain to the full data set, i.e. $\Sigma \equiv \sum_{i=1}^{n}$.

2.2. Baseline shift C

The general solution for the baseline parameter C is readily obtained from the condition that the derivative of χ^2 to C is zero, i.e. $\partial\chi^2/\partial C = 0$

$$\Sigma\sigma_i^{-2} \left(y_i - Ax_i - C \right) = 0 \tag{2.4}$$

which immediately leads to

$$C = y_w - Ax_w \tag{2.5}$$

in which $x_w = \Sigma w_i x_i$ and $y_w = \Sigma w_i y_i$ are the weighted mean values of x and y, respectively, using also for x_i the weighting factor $w_i = \sigma_i^{-2}/\Sigma\sigma_k^{-2}$ associated with the variance of y_i.

2.3. Amplitude A

Equating the derivative of χ^2 to A to zero, $\partial\chi^2/\partial A = 0$,

$$\Sigma\sigma_i^{-2} \left((y_i - y_w) - A(x_i - x_w) \right) (x_i - x_w) = 0 \tag{2.6}$$

yields the general least-squares (LSQ) solution for the amplitude A of the cyclic modulation

$$A = \frac{\Sigma w_i (y_i - y_w)(x_i - x_w)}{\Sigma w_i (x_i - x_w)^2} \tag{2.7}$$

The amplitude can also be expressed as

$$A = \frac{\mathrm{cov}(x, y)}{\mathrm{var}(x)} = \frac{s_{x,y}}{s_x^2} \tag{2.8}$$

in which $s_{x,y}$ is the sample covariance of x and y

$$s_{x,y} = \frac{n_{\mathrm{eff}}}{n_{\mathrm{eff}} - 1} \Sigma w_i (x_i - x_w)(y_i - y_w) \tag{2.9}$$

and s_x^2 is the sample variance of x

$$s_x^2 = \frac{n_{\mathrm{eff}}}{n_{\mathrm{eff}} - 1} \Sigma w_i (x_i - x_w)^2 \tag{2.10}$$

where $n_{\mathrm{eff}} = \left(\Sigma w_i^2 \right)^{-1}$ is the 'effective' sample size for normalised weights ($\Sigma w_i = 1$) [46]. It can be verified that $\mathrm{E}[s_x^2] = \mathrm{var}(x)$, since

$$\begin{aligned} \mathrm{E}\left[\Sigma w_i (x_i - x_w)^2 \right] &= \mathrm{E}\left[\Sigma w_i x_i^2 \right] - \mathrm{E}\left[x_w^2 \right] \\ &= \mathrm{var}(x) + \mathrm{E}[x]^2 - \Sigma w_i^2 \mathrm{var}(x) - \mathrm{E}[x_w]^2 \\ &= \left(1 - \Sigma w_i^2 \right) \mathrm{var}(x) \end{aligned} \tag{2.11}$$

2.4. Phase shift φ

Finding the optimum value for the phase shift through $\partial\chi^2/\partial\varphi = 0$ leads to

$$\Sigma\sigma_i^{-2} \left((y_i - y_w) - A(x_i - x_w) \right) (x_i' - x_w') = 0 \tag{2.12}$$

in which $x_i' = \cos(\omega t_i + \varphi)$ is the derivate of x_i to φ and $x_w' = \Sigma w_i x_i$ is its weighted mean. The solution is found by transforming the sine wave in Eq. (2.1) to a sum of orthogonal functions, using the sum rule $\sin(a \pm b) = \sin(a)\cos(b) \pm \sin(b)\cos(a)$

$$y(t) = Ru + Iv + C \tag{2.13}$$

in which $R = A\sin(\varphi + \tau)$, $I = A\cos(\varphi + \tau)$, $u = \cos(\omega t - \tau)$ and $v = \sin(\omega t - \tau)$, and the LSQ solution for C is $C = y_w - Ru_w - Iv_w$. The angular shift τ is chosen such that $\Delta u = (u - u_w)$ and $\Delta v = (v - v_w)$ are orthogonal, i.e. $\Sigma w_i \Delta u_i \Delta v_i = 0$. This condition is fulfilled when the variances of the Δu_i and Δv_i values reach an extremum, i.e. either a maximum or minimum value. Four solutions for τ can be found within the range $[0, 2\pi]$, each solution differing by a value of $\pi/2$ from the next one. For example, using the derivative of the sum of Δv_i^2 values with weighting factors w_i and applying sum rules

$$\begin{aligned} \frac{\partial \Sigma w_i \Delta v_i^2}{\partial\tau} &= 2\Sigma w_i \Delta v_i \Delta u_i \\ &= 2\left[\Sigma w_i v_i u_i - v_w u_w \right] \\ &= \Sigma w_i \sin\left(2(\omega t_i - \tau) \right) - 2\Sigma w_i \sin\left(\omega t_i - \tau \right) \Sigma w_i \cos\left(\omega t_i - \tau \right) \\ &= \cos(2\tau)\left[s_2 - 2s_1c_1 \right] - \sin(2\tau)\left[c_2 + s_1^2 - c_1^2 \right] = 0 \end{aligned} \tag{2.14}$$

one finds a solution for the angle τ

$$\tau = \frac{1}{2}\tan^{-1}\left[\frac{s_2 - 2s_1c_1}{c_2 + s_1^2 - c_1^2} \right] \tag{2.15}$$

in which

$$\begin{cases} c_1 = \Sigma w_i \cos\left(\omega t_i \right) & c_2 = \Sigma w_i \cos\left(2\omega t_i \right) \\ s_1 = \Sigma w_i \sin\left(\omega t_i \right) & s_2 = \Sigma w_i \sin\left(2\omega t_i \right) \end{cases} \tag{2.16}$$

The Eqs. (2.6) and (2.12) combine into an equivalent set

$$\begin{cases} \Sigma w_i \left[\Delta y_i - R\Delta u_i - I\Delta v_i \right] \left(R\Delta u_i + I\Delta v_i \right) = 0 \\ \Sigma w_i \left[\Delta y_i - R\Delta u_i - I\Delta v_i \right] \left(I\Delta u_i - R\Delta v_i \right) = 0 \end{cases} \tag{2.17}$$

which can be manipulated by summing both equations, after multiplying the 1st and 2nd equation with (R and I) or (–I and R), respectively. Due to the orthogonality, the set reduces to

$$\begin{cases} \Sigma w_i \left(\Delta y_i \Delta u_i - R\Delta u_i^2 \right) = 0 \\ \Sigma w_i \left(\Delta y_i \Delta v_i - I\Delta v_i^2 \right) = 0 \end{cases} \tag{2.18}$$

thus defining R as

$$R = \frac{\Sigma w_i (y_i - y_w)(u_i - u_w)}{\Sigma w_i (u_i - u_w)^2} = \frac{s_{u,y}}{s_u^2} \tag{2.19}$$

and I as

$$I = \frac{\Sigma w_i (y_i - y_w)(v_i - v_w)}{\Sigma w_i (v_i - v_w)^2} = \frac{s_{v,y}}{s_v^2} \tag{2.20}$$

in which $s_{u,y}$, $s_{v,y}$, s_u^2, s_v^2 and n_{eff} are defined in a similar manner as was done for $s_{x,y}$ and s_x^2 in Eqs. (2.9)–(2.10).

The phase shift is calculated as the sum of two angles, $\varphi = \phi - \tau$, with $-\tau$ from Eq. (2.15) and ϕ from

$$\phi = \tan^{-1}\left(\frac{R}{I} \right) = \tan^{-1}\left(\frac{s_{u,y}}{s_u^2} \frac{s_v^2}{s_{v,y}} \right) \tag{2.21}$$

2.5. Variance of A

Ignoring systematic errors which would introduce correlations between uncertainties, the variance of the amplitude A obtained from an inverse-variance weighted LSQ fit with fixed phase φ results in [47–49] (see Section 5.1)

$$\sigma_A^2 = \frac{\Sigma\sigma_i^{-2}}{\Sigma\sigma_i^{-2}\Sigma x_i^2\sigma_i^{-2} - (\Sigma x_i \sigma_i^{-2})^2} \tag{2.22}$$

or, in terms of the variance of the weighted mean y_w and the sample variance of x

$$\sigma_A^2 = \frac{n_{\mathrm{eff}}}{n_{\mathrm{eff}} - 1} \frac{\sigma_{y_w}^2}{s_x^2} \tag{2.23}$$

in which

$$\sigma^2_{y_w} = \left(\Sigma\sigma_i^{-2}\right)^{-1} \tag{2.24}$$

2.6. Normalised amplitude A'

The LSQ fit tends to find solutions for φ where the variance of x is comparably small and A is large (see Section 7 for simulation results). In particular for small data sets, the fitted amplitudes can take extreme values, which may be misinterpreted as statistically significant. The variance of the fitted amplitude is inversely proportional to the sample variance of the x values (Eq. (2.23)). The normalised amplitude A' is made to correspond to a standard width of var(x)=1/2 [14]

$$A' = A\sqrt{2s_x^2} = \frac{s_{x,y}}{\sqrt{s_x^2/2}} \tag{2.25}$$

The variance of the normalised amplitude A' is independent of the spread of the x values and proportional to the variance of the weighted mean y_w

$$\sigma^2_{A'} = \frac{n_{\text{eff}}}{n_{\text{eff}}-1} 2\sigma^2_{y_w} \tag{2.26}$$

Normalised versions of the amplitudes R and I obtained at an angular phase shift $-\tau$ can be defined as

$$R' = R\sqrt{2s_u^2} \quad \text{and} \quad I' = I\sqrt{2s_v^2} \tag{2.27}$$

There is a simple relationship between A' and its matching (R', I') pair for which $A\Delta x = R\Delta u + I\Delta v$, since

$$\Sigma w_i \left(A\Delta x_i\right)^2 = \Sigma w_i (R\Delta u_i + I\Delta v_i)^2 \tag{2.28}$$

and due to the orthogonality of Δu and Δv

$$A^2 \left(\Sigma w_i \Delta x_i^2\right) = R^2 \left(\Sigma w_i \Delta u_i^2\right) + I^2 \left(\Sigma w_i \Delta v_i^2\right) \tag{2.29}$$

which is equivalent to

$$A'^2 = R'^2 + I'^2 \tag{2.30}$$

The normalised amplitude A' follows directly from the squared sum of R' and I'.

3. Weighted LSQ fit ($C = 0$)

3.1. Fit function

Unlike in Eq. (2.1), the fit function in Eq. (3.1) for a sinusoidal modulation in a time series does not contain an offset parameter C

$$y(t) = A\sin(\omega t + \varphi) \tag{3.1}$$

which has implications on the LSQ fit results for the remaining free parameters, being the amplitude A and the phase shift φ. The same result for A and φ as with Eq. (2.1) would be obtained if the x and y data were pre-treated by subtracting x_w and y_w, respectively, however x_w depends on the angle φ. Only in case of a sufficiently large and homogeneous set of x data, can one assume that $x_w \to 0$ for any angle φ. Pre-treatment of the y data suffices to obtain the same amplitude, but there is still a difference in the degrees of freedom affecting the uncertainty and the power (see Section 6).

3.2. Amplitude A

In absence of an offset parameter C, the condition $\partial\chi^2/\partial A = 0$ is equivalent to

$$\Sigma w_i \left(y_i - Ax_i\right) x_i = 0 \tag{3.2}$$

and a modified LSQ solution for the amplitude is obtained

$$A = \frac{\Sigma w_i y_i x_i}{\Sigma w_i x_i^2} \tag{3.3}$$

The amplitude can also be expressed as

$$A = \frac{\text{cov}(x,y)}{\text{var}(x)} = \frac{s'_{x,y}}{s'^2_x} \tag{3.4}$$

in which $s'_{x,y}$ is the sample covariance of x and y

$$s'_{x,y} = \Sigma w_i x_i y_i \tag{3.5}$$

and s'^2_x is the sample variance of x

$$s'^2_x = w_i x_i^2 \tag{3.6}$$

Similarly to the definition in Eq. (2.25), the normalised amplitude is then

$$A' = A\sqrt{2s'^2_x} = \frac{s'_{x,y}}{\sqrt{s'^2_x/2}} \tag{3.7}$$

The variance of the amplitude can be expressed in terms of the variance of the weighted mean y_w and the sample variance of x

$$\sigma^2_A = \frac{\sigma^2_{y_w}}{s'^2_x} \tag{3.8}$$

whereas for the normalised amplitude

$$\sigma^2_{A'} = 2\sigma^2_{y_w} \tag{3.9}$$

3.3. Phase shift φ

Similarly as in Section 2.4, the basic equation is transformed to a sum of orthogonal functions

$$y(t) = Ru + Iv \tag{3.10}$$

in which $R = A\sin(\varphi+\tau)$, $I = A\cos(\varphi+\tau)$, $u = \cos(\omega t - \tau)$ and $v = \sin(\omega t - \tau)$. The angular shift τ is chosen such that u and v are orthogonal, i.e. $\Sigma w_i u_i v_i = 0$. This condition is fulfilled when the spread of the u_i and v_i values reach an extremum

$$\begin{aligned} \frac{\partial \Sigma w_i v_i^2}{\partial \tau} &= 2\Sigma w_i v_i u_i \\ &= 2\Sigma w_i \sin\left(2(\omega t_i - \tau)\right) \\ &= \cos(2\tau)\left[s_2\right] - \sin(2\tau)\left[c_2\right] = 0 \end{aligned} \tag{3.11}$$

which occurs at the angle τ

$$\tau = \frac{1}{2}\tan^{-1}\left[\frac{s_2}{c_2}\right] \tag{3.12}$$

with s_2 and c_2 as defined in Eq. (2.16).

Owing to the orthogonality of u and v, the set of equations $\partial\chi^2/\partial A = 0$ and $\partial\chi^2/\partial\varphi = 0$ is equivalent to

$$\begin{cases} \Sigma w_i \left(y_i u_i - Ru_i^2\right) = 0 \\ \Sigma w_i \left(y_i v_i - Iv_i^2\right) = 0 \end{cases} \tag{3.13}$$

thus defining R and I as

$$R = \frac{\Sigma w_i y_i u_i}{\Sigma w_i u_i} = \frac{s'_{u,y}}{s'^2_u} \tag{3.14}$$

and

$$I = \frac{\Sigma w_i y_i v_i}{\Sigma w_i v_i^2} = \frac{s'_{v,y}}{s'^2_v} \tag{3.15}$$

in which the sample variances are defined in a similar manner as Eqs. (3.5) and (3.6). The phase shift $\varphi = \phi - \tau$ is calculated from τ in Eq. (3.12) and from ϕ in

$$\phi = \tan^{-1}\left(\frac{R}{I}\right) = \tan^{-1}\left(\frac{s'_{u,y}}{s'^2_u}\frac{s'^2_v}{s'_{v,y}}\right) \tag{3.16}$$

The normalised versions of R and I are defined as

$$R' = R\sqrt{2s'^2_u} \quad \text{and} \quad I' = I\sqrt{2s'^2_v} \tag{3.17}$$

Starting from $Ax = Ru + Iv$ and the orthogonality of u and v, it is straightforward to derive the relationship $A'^2 = R'^2 + I'^2$, as was done in Section 2 for Eq. (2.30).

3.4. Sample variances

There is a simple relationship between the different definitions of the sample variances used for C = free and $C = 0$, respectively. Since $\Sigma w_i(x_i - x_w)y_w = 0$, the covariance $s_{x,y}$, as defined in Eq. (2.9), can be written as

$$s_{x,y} = \frac{n_{\text{eff}}}{n_{\text{eff}} - 1}\Sigma w_i(x_i - x_w)y_i = \frac{n_{\text{eff}}}{n_{\text{eff}} - 1}\left[s'_{x,y} - x_w y_w\right] \tag{3.18}$$

and since $\Sigma w_i(x_i - x_w)x_w = 0$, the sample variance s_x^2 from Eq. (2.10) is equivalent to

$$s_x^2 = \frac{n_{\text{eff}}}{n_{\text{eff}} - 1}\left[s_x'^2 - x_w^2\right] \tag{3.19}$$

For data sets with a large degree of freedom ($n_{\text{eff}} \gg 1$) – $n_{\text{eff}}/(n_{\text{eff}}-1) \to 1$, $x_w \to 0$ and $y_w \to 0$ – both versions differ marginally.

4. Unweighted LSQ fit

4.1. Solutions for A , φ and C

In an unweighted fit, the y data carry the same standard uncertainty, $\sigma_i = \sigma_y$, and the weighting factors are identical to w_i=1/n. The mean values x_w and y_w reduce to the arithmetic mean values $\bar{x}$ and $\bar{y}$, and the 'effective' number of data n_{eff} is the sample size n. Specific solutions under these conditions are easily derived from the corresponding general formulas in Sections 2 and 3. For convenience, the solutions for A, φ and C as well as other relevant variables have been collected in the summary Table 1.

4.2. Normalised amplitude A'

The normalised amplitude A' is defined in a similar manner as for weighted fits

$$A' = \begin{cases} \sqrt{2s_x^2}A = \dfrac{s_{x,y}}{\sqrt{s_x^2/2}} & C = \text{free} \\ \sqrt{2s_x'^2}A = \dfrac{s'_{x,y}}{\sqrt{s_x'^2/2}} & C = 0 \end{cases} \tag{4.1}$$

The normalised amplitude A' equals the squared sum of the normalised amplitudes R' and I', as was also the case in Eq. (2.30).

When the phase shift is kept constant in the LSQ fit, e.g. at $\varphi = 0$, the normalised amplitudes A' are normally distributed around 0, and their variance shows a simple relationship with the variance of the y data ($\sigma_i = \sigma_y$) [14]

$$\sigma_{A'}^2 = \begin{cases} \dfrac{2}{n-1}\sigma_y^2 & C = \text{free},\ \varphi = \text{fixed} \\ \dfrac{2}{n}\sigma_y^2 & C = 0, \varphi = \text{fixed} \end{cases} \tag{4.2}$$

which are the unweighted versions of the general formulas in Eqs. (2.26) and (3.9).

5. Statistical distributions

5.1. Gaussian

The amplitude A is the result of a linear fit to normally distributed data y_i and its formula in Eqs. (2.7) or (3.3) is essentially a linear combination of the y values. Consequently, for a fixed angular phase φ, A is normally distributed as well, and its standard deviation σ_A in Eqs. (2.23) or (3.8) is inversely proportional to the standard deviation of x (s_x or s'_x).

The normalised amplitude A' is proportional to A, therefore also follows a normal distribution. Its width has been compensated for the value of s_x or s'_x, such that it corresponds to a standard spread of the x data. At a fixed angular phase shift φ, A' is always drawn from the same normal distribution $\mathcal{N}(0, \sigma_{A'}^2)$.

The same reasoning applies to the amplitudes R and I (Eqs. (2.19)–(2.20) or (3.14)–(3.15)) and their normalised versions R' and I' (Eq. (2.27) or (3.17)), obtained at a 'random' angular phase shift τ. Simulation results are shown in Section 7.

For a particular data set x and a fit with fixed phase ($\varphi = 0$) such that no systematic correlation is created between the x and y data, the variance of A' can be calculated from Eqs. (2.9)–(2.10) and (2.25) for C = free (Eq. (2.1)) and $w_i = \sigma_i^{-2}/\Sigma\sigma_k^{-2}$

$$\sigma_{A'}^2 = \text{Var}\left(\sqrt{2s_x^2}\frac{\Sigma w_i \Delta x_i y_i}{\Sigma w_k \Delta x_k^2}\right) = 2\frac{s_x^2}{\left(\Sigma w_k \Delta x_k^2\right)^2}\Sigma\left(w_i \Delta x_i^2\right)\left(w_i \sigma_i^2\right) = 2\frac{n_{\text{eff}}}{n_{\text{eff}} - 1}\sigma_{y_w}^2 \tag{5.1}$$

since $w_i\sigma_i^2 = (\Sigma\sigma_k^{-2})^{-1} = \sigma_{y_w}^2$. A similar derivation for $C = 0$ (Eq. (3.1)) based on Eqs. (3.5)–(3.7) leads to

$$\sigma_{A'}^2 = 2\text{Var}\left(\frac{\Sigma w_i x_i y_i}{\sqrt{\Sigma w_k x_k^2}}\right) = 2\Sigma\left(\frac{w_i x_i^2}{\Sigma w_k x_k^2}\right)(\Sigma\sigma_k^{-2})^{-1} = 2\sigma_{y_w}^2 \tag{5.2}$$

5.2. Rayleigh

A full scan of the time series for cyclic modulations requires that the phase shift φ is a free fit parameter. As a result, the fit tends to select φ values which yield a non-zero (normalised) amplitude, thus altering the probability density function of A and A'. On the other hand, the angular phase shift τ is correlated with the x data, but can still be interpreted as a 'random' choice with respect to the y data. Therefore, R' and I' are drawn independently from the same normal distribution $\mathcal{N}(0, \sigma_{A'}^2)$. The absolute value of the normalised amplitude A' is the square sum of the normalised amplitudes R' and I'

$$|A'| = \sqrt{R'^2 + I'^2} \tag{5.3}$$

The resulting probability density function for $|A'|$ is a Rayleigh distribution $\mathcal{Rayleigh}(\sigma_{A'})$. It is equivalent to a $\mathcal{Weibull}(\alpha, \beta)$ distribution with $\alpha = 2$ and $\beta = \sqrt{2}\sigma_{A'}$. The mean value of the probability distribution is

$$\text{E}(|A'|) = \sigma_{A'}\sqrt{\frac{\pi}{2}} \approx 1.253\sigma_{A'} \tag{5.4}$$

The mode is $\sigma_{A'}$, and the variance is

$$\text{var}(|A'|) = \left(2 - \frac{\pi}{2}\right)\sigma_{A'}^2 \approx 0.429\sigma_{A'}^2 \tag{5.5}$$

5.3. Exponential

Given that $k = |A'|/\sigma_{A'}$ is $\mathcal{Rayleigh}(1)$-distributed, its squared value k^2 follows a chi-squared distribution with $N = 2$ degrees of freedom, $k^2 \sim \chi^2(2)$. Its cumulative distribution is $F(x; N = 2) = 1 - e^{-x/2}$. Consequently, the probability that $|A'|$ exceeds a value $k\sigma_{A'}$ follows an exponential distribution $\mathcal{Exp}(1/2)$

$$\text{P}(|A'| > k\sigma_{A'}) = \text{e}^{-k^2/2} \tag{5.6}$$

This significance test shows a simple relationship with the ratio of the normalised height $|A'|$ of the sinusoidal cycle relative to the standard

Table 1
Equations resulting from LSQ fitting of a cyclic modulation to normally-distributed white noise, either for weighted or unweighted fits, with or without a baseline shift C. Some definitions of variables are repeated here: $x_i = \sin(\omega t_i + \varphi)$, $x_w = \Sigma w_i x_i$, $\overline{x} = \Sigma x_i / n$, $u_i = \cos(\omega t_i - \tau)$, $v_i = \sin(\omega t_i - \tau)$, $s_j = \Sigma w_i \sin\left(j\omega t_i\right)$ and $c_j = \Sigma w_i \cos\left(j\omega t_i\right)$ for $j \in \{1,2\}$.

	Weighted fit		Unweighted fit	
	$y(t) = A\sin(\omega t + \varphi) + C$	$y(t) = A\sin(\omega t + \varphi)$	$y(t) = A\sin(\omega t + \varphi) + C$	$y(t) = A\sin(\omega t + \varphi)$
Normalised weight w_i	$\sigma_i^{-2}/\Sigma\sigma_k^{-2}$	$\sigma_i^{-2}/\Sigma\sigma_k^{-2}$	$1/n$	$1/n$
Effective sample size	$n_{\text{eff}} - 1 = \left(\Sigma w_i^2\right)^{-1} - 1$	$n_{\text{eff}} = \left(\Sigma w_i^2\right)^{-1}$	$n-1$	n
Offset C	$C = y_w - A x_w$	0	$C = \overline{y} - A\overline{x}$	0
Amplitude A	$\frac{\Sigma w_i (y_i - y_w)(x_i - x_w)}{\Sigma w_i (x_i - x_w)^2}$	$\frac{\Sigma w_i y_i x_i}{\Sigma w_i x_i^2}$	$\frac{\Sigma (y_i - \overline{y})(x_i - \overline{x})}{\Sigma (x_i - \overline{x})^2}$	$\frac{\Sigma y_i x_i}{\Sigma x_i^2}$
Amplitude A	$\frac{s_{x,y}}{s_x^2}$	$\frac{s'_{x,y}}{s_x'^2}$	$\frac{s_{x,y}}{s_x^2}$	$\frac{s'_{x,y}}{s_x'^2}$
Sample cov $s_{x,y}$	$\frac{n_{\text{eff}}}{n_{\text{eff}} - 1} \Sigma w_i (x_i - x_w)(y_i - y_w)$	$\Sigma w_i x_i y_i$	$\frac{1}{n-1} \Sigma (x_i - \overline{x})(y_i - \overline{y})$	$\frac{1}{n} \Sigma x_i y_i$
Sample width s_x^2	$\frac{n_{\text{eff}}}{n_{\text{eff}} - 1} \Sigma w_i (x_i - x_w)^2$	$\Sigma w_i x_i^2$	$\frac{1}{n-1} \Sigma (x_i - \overline{x})^2$	$\frac{1}{n} \Sigma x_i^2$
Normalised A'	$\sqrt{2 s_x^2} A = \frac{s_{x,y}}{\sqrt{s_x^2/2}}$	$\sqrt{2 s_x'^2} A = \frac{s'_{x,y}}{\sqrt{s_x'^2/2}}$	$\sqrt{2 s_x^2} A = \frac{s_{x,y}}{\sqrt{s_x^2/2}}$	$\sqrt{2 s_x'^2} A = \frac{s'_{x,y}}{\sqrt{s_x'^2/2}}$
Variance $\sigma_{A'}^2$	$2\sigma_{y_w}^2 \frac{n_{\text{eff}}}{n_{\text{eff}} - 1}$	$2\sigma_{y_w}^2$	$2\sigma_{\overline{y}}^2 \frac{n}{n-1}$	$2\sigma_{\overline{y}}^2$
Variance $\sigma_{y_w}^2$, $\sigma_{\overline{y}}^2$	$\left(\Sigma\sigma_i^{-2}\right)^{-1}$	$\left(\Sigma\sigma_i^{-2}\right)^{-1}$	σ_y^2/n	σ_y^2/n
Power $S = \frac{1}{2}\frac{A'^2}{\sigma_{A'}^2}$	$\left[\frac{\Sigma\sigma_i^{-2}}{2} \frac{n_{\text{eff}} - 1}{n_{\text{eff}}}\right] \left[\frac{s_{x,y}^2}{s_x^2}\right]$	$\left[\frac{\Sigma\sigma_i^{-2}}{2}\right] \left[\frac{s_{x,y}'^2}{s_x'^2}\right]$	$\left[\frac{1}{2} \frac{n-1}{\sigma_y^2}\right] \left[\frac{s_{x,y}^2}{s_x^2}\right]$	$\left[\frac{1}{2} \frac{n}{\sigma_y^2}\right] \left[\frac{s_{x,y}'^2}{s_x'^2}\right]$
Orthogonal angle τ	$\frac{1}{2}\tan^{-1}\left[\frac{s_2 - 2 s_1 c_1}{c_2 + s_1^2 - c_1^2}\right]$	$\frac{1}{2}\tan^{-1}\left[\frac{s_2}{c_2}\right]$	$\frac{1}{2}\tan^{-1}\left[\frac{s_2 - 2 s_1 c_1}{c_2 + s_1^2 - c_1^2}\right]$	$\frac{1}{2}\tan^{-1}\left[\frac{s_2}{c_2}\right]$
Amplitude R	$\frac{s_{u,y}}{s_u^2}$	$\frac{s'_{u,y}}{s_u'^2}$	$\frac{s_{u,y}}{s_u^2}$	$\frac{s'_{u,y}}{s_u'^2}$
Amplitude I	$\frac{s_{v,y}}{s_v^2}$	$\frac{s'_{v,y}}{s_v'^2}$	$\frac{s_{v,y}}{s_v^2}$	$\frac{s'_{v,y}}{s_v'^2}$
Phase $\phi = \varphi + \tau$	$\tan^{-1}\left(\frac{s_{u,y}}{s_u^2}\frac{s_v^2}{s_{v,y}}\right)$	$\tan^{-1}\left(\frac{s'_{u,y}}{s_u'^2}\frac{s_v'^2}{s'_{v,y}}\right)$	$\tan^{-1}\left(\frac{s_{u,y}}{s_u^2}\frac{s_v^2}{s_{v,y}}\right)$	$\tan^{-1}\left(\frac{s'_{u,y}}{s_u'^2}\frac{s_v'^2}{s'_{v,y}}\right)$
Normalised R'	$\sqrt{2 s_u^2} R = \frac{s_{u,y}}{\sqrt{s_u^2/2}}$	$\sqrt{2 s_u'^2} R = \frac{s'_{u,y}}{\sqrt{s_u'^2/2}}$	$\sqrt{2 s_u^2} R = \frac{s_{u,y}}{\sqrt{s_u^2/2}}$	$\sqrt{2 s_u'^2} R = \frac{s'_{u,y}}{\sqrt{s_u'^2/2}}$
Normalised I'	$\sqrt{2 s_v^2} I = \frac{s_{v,y}}{\sqrt{s_v^2/2}}$	$\sqrt{2 s_v'^2} I = \frac{s'_{v,y}}{\sqrt{s_v'^2/2}}$	$\sqrt{2 s_v^2} I = \frac{s_{v,y}}{\sqrt{s_v^2/2}}$	$\sqrt{2 s_v'^2} I = \frac{s'_{v,y}}{\sqrt{s_v'^2/2}}$
Power $S = \frac{1}{2}\frac{R'^2 + I'^2}{\sigma_{A'}^2}$	$\left[\frac{1}{2}\sigma_{y_w}^{-2}\frac{n_{\text{eff}} - 1}{n_{\text{eff}}}\right]\left[\frac{s_{u,y}^2}{s_u^2} + \frac{s_{v,y}^2}{s_v^2}\right]$	$\left[\frac{1}{2}\sigma_{y_w}^{-2}\right]\left[\frac{s_{u,y}'^2}{s_u'^2} + \frac{s_{v,y}'^2}{s_v'^2}\right]$	$\left[\frac{1}{2}\sigma_{\overline{y}}^{-2}\frac{n-1}{n}\right]\left[\frac{s_{u,y}^2}{s_u^2} + \frac{s_{v,y}^2}{s_v^2}\right]$	$\left[\frac{1}{2}\sigma_{\overline{y}}^{-2}\right]\left[\frac{s_{u,y}'^2}{s_u'^2} + \frac{s_{v,y}'^2}{s_v'^2}\right]$

uncertainty $\sigma_{A'}$. The inverse cumulative distribution or quantile function Q(p) can be used to determine k such that there is a probability $1 - p$ that a value $|A'| > k\sigma_{A'}$ is generated from normally distributed noise

$$k = \mathrm{Q}(p)/\sigma_{A'} = \sqrt{-2\ln(1-p)} \tag{5.7}$$

If the power S is defined as

$$S = \frac{1}{2}\left(\frac{A'}{\sigma_{A'}}\right)^2 = \frac{1}{2}k^2 \tag{5.8}$$

then S is $\mathcal{E}xp(1)$-distributed with expected value E[S]=1 and variance Var[S]=1 and the significance test is simply P($power > S$) = e^{-S}. The value of S which corresponds to a probability $1 - p$ that the generated power is larger than S is calculated from

$$S = \mathrm{Q}(p) = -\ln(1-p) \tag{5.9}$$

6. Lomb–Scargle periodogram

6.1. Amplitudes R and I

The L–S solution [5,7] is equivalent to a least squares fit of a function

$$y(t) = Ru + Iv \tag{6.1}$$

in which τ is the angle at which $u = \cos(\omega t - \tau)$ and $v = \sin(\omega t - \tau)$ are orthogonal. In the classical L–S periodogram, the baseline C is zero, the standard deviation $\sigma_i = \sigma_y$ is assumed to be constant (and known *a priori*) for all data, and the weighting factors are identical to $w_i = 1/n$. Without additional difficulty, it can be upgraded to a weighted fit with $w_i = \sigma_i^{-2}/\Sigma\sigma_k^{-2}$.

The least squares solutions for R and I are easily found under the condition that the sum of cross terms Σuv is zero (Eq. (3.11)). For example:

$$\begin{aligned} \frac{\partial\chi^2}{\partial R} &= \frac{\partial\Sigma w_i (y_i - Ru_i - Iv_i)^2}{\partial R} \\ &= -2\Sigma w_i (y_i - Ru_i - Iv_i) u_i \\ &= -2\left(\Sigma w_i y_i u_i - R\Sigma w_i u_i^2\right) = 0 \end{aligned} \tag{6.2}$$

The resulting equations for R and I are the same as Eqs. (3.14)–(3.15), therefore $R = A\sin(\varphi+\tau)$, $I = A\cos(\varphi+\tau)$ and τ is defined in Eq. (3.12). The quadratic sum of the amplitudes equals $A^2 = R^2 + I^2$. The same relationship holds for the normalised amplitudes, $A'^2 = R'^2 + I'^2$, as already deduced in Sections 2 and 3.

6.2. Amplitude A and angle φ

The Lomb–Scargle solution in Eq. (6.1) should match exactly with the LSQ solution in Eq. (3.1) (for $C = 0$) for a single sinusoidal function, i.e. $Ax = Ru + Iv$. This implies a simple relationship between the amplitudes

$$|A| = \sqrt{R^2 + I^2} \tag{6.3}$$

and the angles

$$\phi = \varphi + \tau = \begin{cases} \pi/2 & R = 0, I \geq 0 \\ \tan^{-1}\left(\frac{R}{I}\right) & R \neq 0 \\ -\pi/2 & R = 0, I < 0 \end{cases} \tag{6.4}$$

such that

$$|A| \sin(\omega t + \varphi) = \sqrt{R^2 + I^2}\,\mathrm{sgn}(I) \sin(\omega t + \phi - \tau) \tag{6.5}$$

in which sgn(I) takes the value of +1 if $I > 0$ and −1 if $I < 0$.

6.3. Power ($C = 0$)

The 'power' associated with the L–S solution for an angular period ω is said [7] to equal half the gain in the sum of squares ($C = 0$)

$$\begin{aligned} S(\omega) &= \frac{1}{2}\left(\chi_0^2 - \chi_\omega^2\right) \\ &= \frac{1}{2}\left[\Sigma\left(\frac{y_i - 0}{\sigma_i}\right)^2 - \Sigma\left(\frac{y_i - Ax_i}{\sigma_i}\right)^2\right] \\ &= \frac{1}{2}\left[\Sigma\sigma_i^{-2}\left(2y_i(Ax_i) - (Ax_i)^2\right)\right] \\ &= \frac{1}{2}\left(\Sigma\sigma_k^{-2}\right)\left[A^2 \Sigma w_i x_i^2\right] \\ &= \frac{1}{2}\frac{\left[2A^2 s_x'^2\right]}{\left[2\sigma_{y_w}^2\right]} = \frac{1}{2}\frac{A'^2}{\sigma_{A'}^2} = \frac{k^2}{2} \end{aligned} \tag{6.6}$$

in which use was made of Eq. (3.2). The outcome of Eq. (6.6) – i.e. in the case of $C = 0$ – is indeed identical to the definition of the power given in Eq. (5.8). Based on Eq. (2.30), the power in Eq. (6.6) can be expressed as

$$\begin{aligned} S(\omega) &= \frac{1}{2}\frac{R'^2 + I'^2}{\sigma_{A'}^2} \\ &= \frac{1}{2}\sigma_{y_w}^{-2}\left[\frac{s_{u,y}'^2}{s_u'^2} + \frac{s_{v,y}'^2}{s_v'^2}\right] \end{aligned} \tag{6.7}$$

In the unweighted case ($w_i = 1/n$), one finds

$$S(\omega) = \frac{1}{2\sigma_y^2}\left[\frac{\left(\Sigma y_i u_i\right)^2}{\Sigma u_i^2} + \frac{\left(\Sigma y_i v_i\right)^2}{\Sigma v_i^2}\right] \tag{6.8}$$

This is equivalent to the definition given by Scargle [7], except for an additional factor σ_y^{-2} which was missing because he normalised the variance of the time series ($\sigma_y^2 = 1$). The power criterion of the L–S periodogram is equivalent to the significance test of the LSQ solution in Eq. (5.6).

6.4. Power ($C \neq 0$)

The trick with half the gain in the sum of squares does not work as a means to determine the power when the baseline parameter C is fitted freely. An adjustment needs to be made to the initial value of the chi square, replacing y_i values by Δy_i, and a correction factor has to be introduced for decreasing the degrees of freedom by one

$$\begin{aligned} S(\omega) &= \frac{1}{2}\frac{n_{\mathrm{eff}}}{n_{\mathrm{eff}} - 1}\left(\chi_1^2 - \chi_\omega^2\right) \\ &= \frac{1}{2}\frac{n_{\mathrm{eff}}}{n_{\mathrm{eff}} - 1}\left[\Sigma\left(\frac{\Delta y_i}{\sigma_i}\right)^2 - \Sigma\left(\frac{\Delta y_i - A\Delta x_i}{\sigma_i}\right)^2\right] \\ &= \frac{1}{2}\left(\Sigma\sigma_k^{-2}\right)\left[A^2 \frac{n_{\mathrm{eff}}}{n_{\mathrm{eff}} - 1}\Sigma w_i \Delta x_i^2\right] \\ &= \frac{1}{2}\frac{\left[2A^2 s_x^2\right]}{\left[2\sigma_{y_w}^2\right]} = \frac{1}{2}\frac{A'^2}{\sigma_{A'}^2} = \frac{k^2}{2} \end{aligned} \tag{6.9}$$

6.5. Pre-treatment of data

It has been mentioned in Section 3, that the data set can be pre-treated by replacing y_i with $\Delta y_i = y_i - y_w$ and then fed into the equations for $y(t) = Ax$ (Section 3) instead of $y(t) = Ax - C$ (Section 2). The analysis for $C = 0$ would yield the same amplitudes A as for C=free, albeit it with different φ values. By applying a correction factor for the change in degrees of freedom due to subtracting a mean value, the correct power is obtained

$$S_{y(t)=Ax+C} = \frac{n_{\mathrm{eff}}}{n_{\mathrm{eff}} - 1} S_{y(t)=Ax} \tag{6.10}$$

7. Simulations

7.1. Data sets x, y

Eighty thousand simulations were performed of LSQ fits of Eqs. (2.1) and (3.1) to white noise. The x data were generated from uniformly distributed time t values over a full period. Three types of y data sets were generated from normal distributions $\mathcal{N}(0, \sigma_i^2)$

- Set 1: $\sigma_i = \{1, 2, 2\}$, $n = 3$, $n_{\mathrm{eff}} = 2$, $\sigma_{A'} = \left\{\sqrt{4/3}, \sqrt{8/3}\right\}$
- Set 2: $\sigma_i = \{1, 1, 1\}$, $n = 3$, $n_{\mathrm{eff}} = 3$, $\sigma_{A'} = \left\{\sqrt{2/3}, 1\right\}$
- Set 3: $\sigma_i = \{17 \times 1, 21 \times 2, 12 \times 3\}$, $n = 50$, $n_{\mathrm{eff}} = 30.128$, $\sigma_{A'} = \{0.291, 0.296\}$

The $\sigma_{A'}^2$ values are obtained from Eq. (3.9) for $C = 0$, and from Eq. (2.26) for C = free, respectively.

7.2. Amplitude R', I', A'

The probability distributions of the fitted amplitudes R', I', and A' are shown in Fig. 1. The normalised amplitudes R' and I' are not correlated with the y values and follow the expected $\mathcal{N}(0, \sigma_{A'}^2)$ distribution. The composite amplitude A' is $\mathcal{Rayleigh}(\sigma_{A'})$-distributed, as expected in Section 5.2. Owing to the introduction of the 'effective' sample size n_{eff}, the equations are also rigorously applicable to unequally weighted fits, for which $n_{\mathrm{eff}} \neq n$.

7.3. Erratum

In Ref. [14], simulations were performed of unweighted LSQ fits of Eqs. (2.1) and (3.1), and graphs were shown of the statistical distributions of A' for data sets with n = 3, 8 and 50. The Gaussian ($\varphi = 0$) and Rayleigh (φ = free) distributions were perfectly reproduced for C = free, yet somewhat distorted for $C = 0$. This was due to the way the variance of x was calculated to convert A into A', using the Excel function stdev(x) which is equivalent to s_x, but deviates somewhat from s'_x (see Eq. (3.19)).

7.4. Power S

Since A' is $\mathcal{Rayleigh}(\sigma_{A'})$-distributed, it is true that the power $S = k^2/2$ in Eq. (5.8) is $\mathcal{Exp}(1)$-distributed (see Section 5.3). This is confirmed in Fig. 2, showing a similar exponential distribution for all simulations.

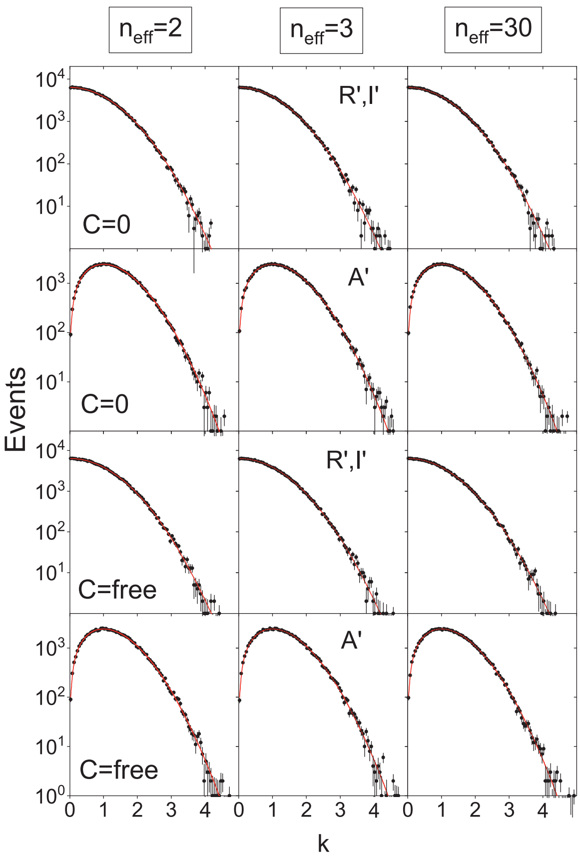

Fig. 1. Frequency distribution of the normalised amplitudes $k = A'/\sigma_{A'}$, $R'/\sigma_{A'}$, and $I'/\sigma_{A'}$ obtained from weighted fits of a cyclic modulation – either through Eq. (3.1) for $C = 0$ or Eq. (2.1) for C = free – to sets of $(n, n_{eff}) = \{(3,2),(3,3),(50,30)\}$ white noise data (see Section 7.1). The red curves indicate the theoretical distributions.

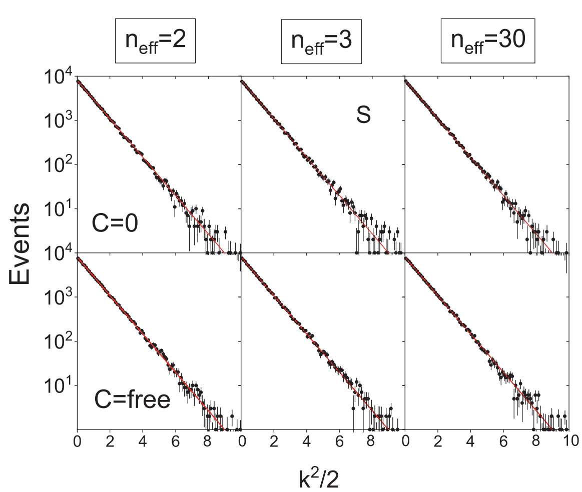

Fig. 2. Frequency distribution of the power $S = k^2/2$ (Eq. (5.8)) obtained from weighted fits of a cyclic modulation – either through Eq. (3.1) for $C = 0$ or Eq. (2.1) for C = free – to sets of $(n, n_{eff}) = \{(3,2),(3,3),(50,30)\}$ white noise data (see Section 7.1). The red curves indicate the theoretical distributions.

7.5. Angle ϕ

Whereas the angles φ and τ are uniformly distributed, their sum $\phi = \varphi + \tau$ is not. From Fig. 3 it is clear that ϕ (modulo π) takes values close to 0 or $\pm\pi/2$, i.e. close to solutions for the angle τ indicating extreme values in the dispersion of u and v. Defining τ_{min} as the τ value

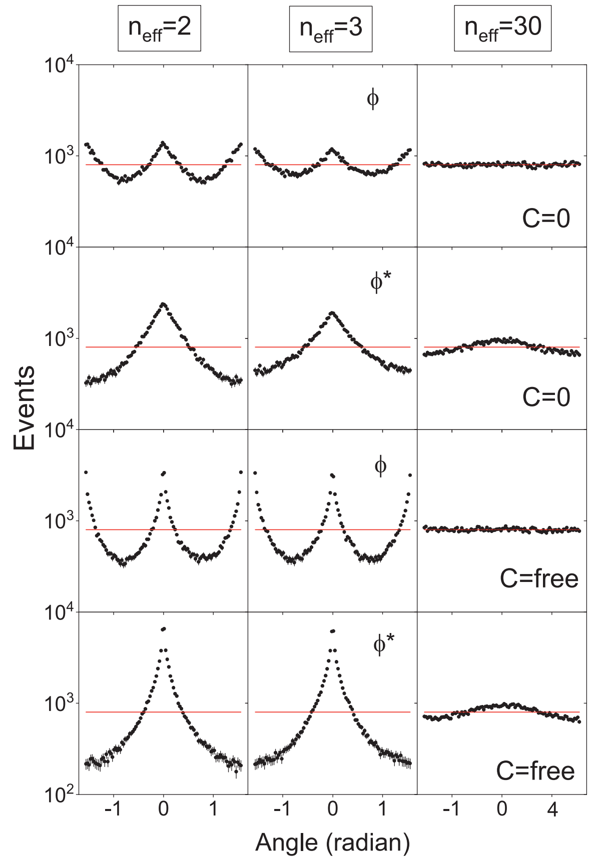

Fig. 3. Frequency distribution of the angles $\phi = \varphi + \tau$ and $\phi^* = \varphi + \tau_{min}$ obtained from weighted fits of a cyclic modulation – either through Eq. (3.1) for $C = 0$ or Eq. (2.1) for C = free – to sets of $(n, n_{eff}) = \{(3,2),(3,3),(50,30)\}$ white noise data (see Section 7.1). The red lines correspond to uniform distributions.

corresponding with $\min(s_u^2)$ – i.e. $\tau_{min} = \tau \pm \pi/2$ if τ indicates $\max(s_u^2)$ – it turns out that $\phi^* = \varphi + \tau_{min}$ (modulo π) is centred around 0. The LSQ fit is attracted to solutions with low dispersion in x – i.e. $\varphi \to -\tau_{min}$ and $s_x^2 \to \min(s_u^2)$ – because this generally leads to larger values of the normalised amplitude through Eqs. (2.25) or (3.7), a high power through Eq. (5.8) and ultimately a low χ^2_ω through Eqs. (6.6) or (6.9). The smaller the data set, the more gain is made from φ approaching $-\tau_{min}$. For the examples shown in Fig. 3, the effect is the largest for $n = 3$ and C = free, both for $n_{eff} = 2$ and 3, because the degree of freedom is zero and $\chi^2_\omega = 0$. For $n_{eff} = 30$, there is still a visible attraction of ϕ^* towards 0.

8. Conclusions

Analytical equations have been derived for the statistical significance of sinusoidal modulations fitted to normally distributed time series. They are based on the ratio of the normalised amplitude A' to its standard deviation parameter $\sigma_{A'}$. The relevant equations are summarised in Table 1. The significance criterion $P = e^{-k^2/2}$ in Eq. (5.6) is universally valid for weighted and unweighted fits, either with or without a free baseline shift parameter C. It is equivalent with the power criterion of the Lomb–Scargle periodogram for $C = 0$. However, when C is a free fit parameter, precautions are needed when deriving the power from the change in the χ^2 of the fit, or when power formulas for $C = 0$ are used in combination with a pre-treated data set in which a mean value is subtracted.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

CRediT authorship contribution statement

S. Pommé: Conceptualization, Methodology, Software, Validation, Formal analysis, Investigation, Writing - original draft, Visualization.

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