Confidence regions for spectral peak frequencies

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A procedure is proposed to obtain confidence regions for spectral peak frequencies. The method is based on resampling the periodogram from the estimated spectrum in order to reestimate the spectrum and its peak frequency. We investigate the dependence of the results from the applied spectral estimator in three simulation studies and apply the method to tremor data.

1 Introduction

Spectral analysis is widely applied to investigate oscillatory phenomena in basic medical and biological research (Marsden et al., 1969; Nelson et al., 1979; Hermann, 1982; Günther, Brunner and Klußmann, 1983; Cleeves and Findley, 1987; Hefter et al., 1987; Beuter and De Geoffroy, 1996; Pinna, Maestri, Di Cesare, 1996; Khutorskaya and Fjodorova, 1996) and clinical diagnosis (Deuschl et al., 1996; Muzi and Ebert, 1993). Often, the power of the oscillation and the peak frequency are of major interest. In general, the spectrum and the peak frequency of a stationary stochastic process are a complicated function of the parameters of the process and can not be expressed analytically. Analytical formulas are known for special classes like the linear autoregressive moving average processes.

Especially in clinical diagnosis it is desirable to decide whether an observed peak frequency is significantly different from the range of peak frequencies obtained from an ensemble of healthy subjects, indicating a pathology. We propose a procedure to obtain such a confidence region. This procedure is based on an heuristic idea, inspired by the parametric bootstrap (Efron and Tibshirani, 1993) and the theory of spectral estimation (Brockwell and Davis, 1987). We investigate its behavior in two simulation studies. General aspects of bootstrapping in the frequency domain are discussed in Franke and Härdle (1992), Janas and Dahlhaus (1994) and Dahlhaus and Janas (1995). Bootstrapping procedures to obtain a confidence region for the mode of densities are discussed in Romano (1988). In the next section we briefly summarize parts of the theory of spectral estimation which are necessary for the proposed procedure introduced in Section 3. In Section 4 three simulation studies are reported which investigate the dependence of the resulting confidence region on the spectral estimator. An application to tremor data is given in Section 5.

2 Spectral estimation

The spectrum $\mathrm{S}(\omega)_{\omega\in(-\pi,\pi)}$ of a stationary stochastic process $X(t)_{t\in\mathbf{Z}}$ is defined as the Fourier transform of the autocovariance function $\mathrm{ACF}(\tau)$:

$$\begin{aligned}\mathrm{ACF}(\tau) &= E(X(t)\,X(t+\tau)) &(1)\\ \mathrm{S}(\omega) &= \frac{1}{2\pi}\sum_{\tau}\mathrm{ACF}(\tau)\exp{(i\,\omega\,\tau)} &(2)\end{aligned}$$

where "$E(.)$" denotes expectation (Brockwell and Davis, 1987). The autocovariance function is assumed to be absolutely summable. The estimation of the spectrum is usually based on the Fourier transform $\mathrm{f}(\omega)$ and the periodogram $\mathrm{Per}(\omega)$ of the data $x(t)_{t=1,\ldots,N}$ (which are usually tapered in order to reduce spectral leakage) :

$$\begin{aligned}\mathrm{f}(\omega) &= \frac{1}{\sqrt{N}}\sum_{t=1}^{N}x(t)\,\exp{(i\,\omega\,t)} &(3)\\ \mathrm{Per}(\omega) &= |\,\mathrm{f}(\omega)\,|^2 &(4)\end{aligned}$$

The periodogram is evaluated for the frequencies :

$$\omega_k=\frac{2\pi k}{N},\quad k=0,\ldots,\frac{N}{2} \qquad . \qquad (5)$$

For two different frequencies ω_1 and ω_2, the values $\mathrm{Per}(\omega_1)$ and $\mathrm{Per}(\omega_2)$ are asymptotically independent. For $\omega\notin\{0,\pi\}$ the periodogram is asymptotically distributed as

$$\frac{1}{2\pi}\mathrm{Per}(\omega)\sim\frac{1}{2}\mathrm{S}(\omega)\,\chi^2_2 \qquad . \qquad (6)$$

Thus, the expectation of the periodogram is the spectrum but the periodogram is not a consistent estimator for the spectrum. In order to estimate the spectrum consistently, the periodogram has to be smoothed by a window function W_j :

$$\widehat{\mathrm{S}}(\omega_k)=\frac{1}{2\pi}\sum_{j=-h}^{h}W_j\,\mathrm{Per}(\omega_{k+j}) \quad ,\ \sum_{j=-h}^{h}W_j=1 \quad , \qquad (7)$$

General aspects of spectral estimation concerning the choice of the window function W_j and its width $2h+1$ as well as other procedures to estimate spectra are given in Brockwell and Davis (1987). To determine global optimal values of h, there exist bootstrap and cross-validation procedures (Faraway and Myoungshic, 1990) as well as data driven methods using a frequency dependent width of the smoothing window (Timmer, Lauk and Deuschl, 1996). The latter two-step algorithm was developed for an optimal estimation of the spectrum in the region of the main peak. First, the width of the main peak is estimated from a spectrum obtained by uniform smoothing. In a second step, based on the estimated width of the peak, a frequency dependent width of the smoothing window is chosen. The width of the kernel at the peak frequency ω_{peak} is proportional the width of the peak. This reflects the fact, that the curvature of the spectrum at ω_{peak} is reciprocally related to the width of the peak. The higher higher curvature the less smoothing is optimal. The width of the kernel increases linearly with $|\omega - \omega_{peak}|$ up to some maximum value.

We do not discuss these algorithms in detail here but show the dependence of the resulting confidence intervals on the smoothing procedure in Section 4 below.

3 The algorithm

The procedure to obtain a confidence region for the estimated peak frequency is given by :

(1) Estimate the spectrum.

(2) Simulate numerous periodograms from the estimated spectrum according to eq. (6).

(3) For each of the simulated periodograms reestimate the spectrum by eq. (7) and the peak frequency.

(4) Obtain the confidence region from the quantiles of the empirical distribution of these estimated peak frequencies.

Denoting the true peak frequency by λ_0, the peak frequency of spectrum estimated from the data by $\hat{\lambda}$ and that of the reestimated spectra by $\hat{\lambda}^*$, the proposed procedure approximates the distribution of $\hat{\lambda} - \lambda_0$ by $\hat{\lambda}^* - \hat{\lambda}$.

For two fixed frequencies the values of the periodogram are asymptotically independent. Two adjacent values of the periodogram might show correlations independent of the number of data points depending on the true spectrum and the tapering window applied (Brockwell and Davis, 1987). The procedure does not take these correlations into account since they decay rapidly within some frequency bins and the smoothing according to eq. (7) usually involves more frequency bins than that correlation length.

In the case of nonlinear or non-Gaussian processes, there might be higher order correlations, e.g. triple correlations described by the bispectrum (Nikias and Mysore, 1987). For oscillatory, i.e. non chaotic, processes these higher order correlations usually appear for harmonically related peaks. Since the proposed procedure only considers the distribution of the periodogram in the neighborhood of the single peak of maximum power, these correlations have not to be taken into account.

4 Simulation Studies

For the simulation studies we choose processes inspired by data of human hand tremor. For treatment monitoring and analysis of temporal fluctuations of tremor, confidence regions of spectral peaks are of special importance.

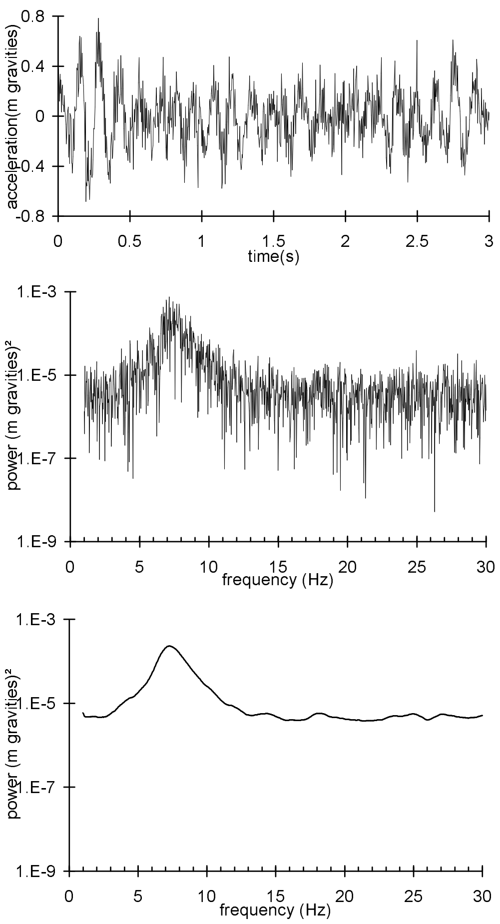

Figure 1: Representative data, the periodogram and estimated spectrum of a physiological hand tremor time series.

Fig. 1 shows a typical time series, the periodogram and the estimated spectrum of a time series obtained from a physiological human hand tremor. Fig. 2 shows the corresponding plots for a time series obtained from a patient suffering from Parkinson's disease. Obviously, apart from the number of frequency bins entering the spectral estimation, the obtainable precision of the estimated peak frequency depends on the curvature of the spectrum at the peak.

The behavior of the proposed procedure will be investigated in three simulation studies which are inspired from the tremor data shown in Fig. 1 and 2. Apart from the above mentioned curvature of the true spectrum the smoothing window used to estimate the spectrum according to eq. (7) will determine the confidence region. The optimal width of the smoothing window de-

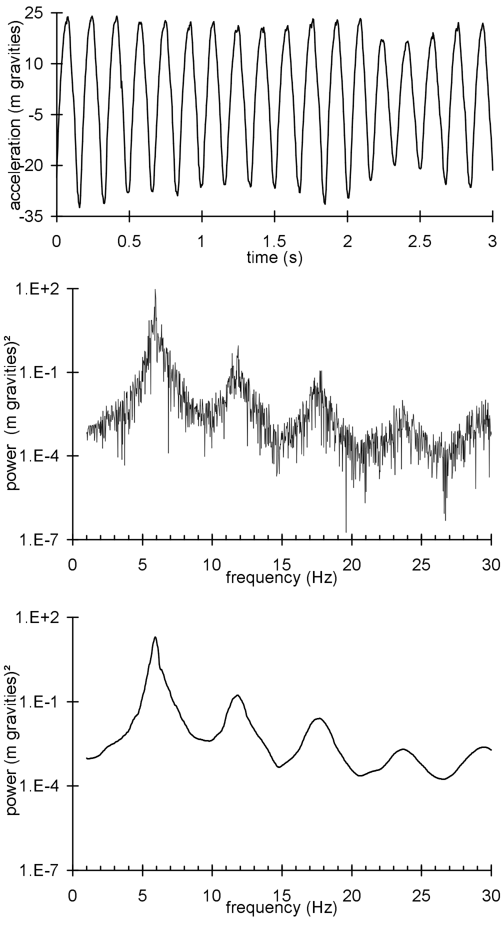

Figure 2: Representative data, the periodogram and estimated spectrum of a Parkinsonian hand tremor time series.

pends on the true spectrum. Therefore, we apply rectangular Daniell windows of different widths as well as the data driven adaptive procedure to choose a frequency dependent width which has been described in Timmer et al. (1996). Each simulated time series consists of 10000 data points. This is a typical amount of data in tremor measurements and also for other electrophysiological applications like EEG or ECG. For each simulation study the bias and the variance of the estimator for the peak frequency and the coverage probability is estimated. The resampling procedure described above uses 500 simulated periodograms, where 90 % confidence intervals based on the lower and upper 5 % quantiles are considered only. Each simulation study consists of 500 repetitions, too.

In order to treat the problem of choosing confidence intervals for the discrete distribution on the frequency bins, there exist three possibilities:

- The two bins where the 5 % and 95 % quantiles are located are included in the confidence region.
- Out of the three possible combinations (include both bins, left or right bin) that one is chosen, that leads to the least conservative confidence region.
- A randomized confidence region is chosen (Stuart, 1991).

Here, we chose the first possibility.

The physiological tremor is well described by a linear stochastic autoregressive (AR) process (Randall, 1973; Gantert, Honerkamp and Timmer, 1992). An AR process of order p is given by :

$$x(t) = \sum_{i=1}^{p} a_i \, x(t-i) \, + \, \epsilon(t) \quad , \tag{8}$$

where $\epsilon(t)$ denotes i.i.d. Gaussian random variables with mean zero and variance σ^2. Such a process can be interpreted in terms of physics depending on the chosen parameters as a combination of relaxators and damped oscillators (Honerkamp, 1993). For example, in the case of an AR process of order 2 with appropriate chosen parameters a_1 and a_2, the process describes a damped linear oscillator. The characteristic period T and relaxation time τ are related to the parameters by:

$$a_1 = 2\cos\left(\frac{2\pi}{T}\right)\exp\left(-1/\tau\right) \tag{9}$$

$$a_2 = -\exp\left(-2/\tau\right) \quad . \tag{10}$$

The spectrum is given by :

$$\mathrm{S}(\omega) = \frac{1}{2\pi}\frac{\sigma^2}{|1 - a_1 e^{-i\omega} - a_2 e^{-2i\omega}|^2} \tag{11}$$

and the peak frequency is located at :

$$\omega_{peak} = \arccos\left(\cos(2\pi/T)\,\cosh(1/\tau)\right) \tag{12}$$

The width of the peak $\Delta\ \omega$ can be measured by the difference of the frequencies where the power decreased to half the value at the peak. This half power width of the peak is monotonically related to $1/\tau$.

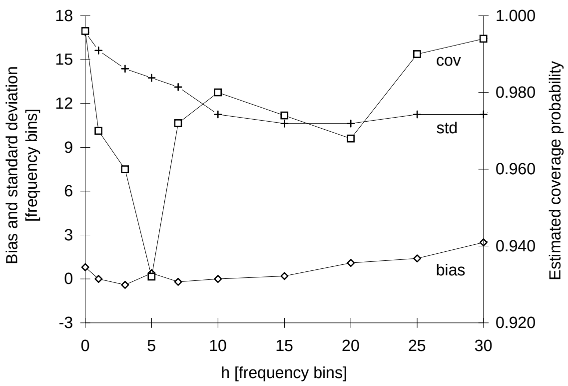

Figure 3: Result of the simulation study for an AR [2] process with $T = 50$ and $\tau = 100$. Shown is the dependence of the bias ($\diamond$), standard deviation ($+$) of the estimator for the peak frequency and the coverage probability ($\square$) on the width of the smoothing window.

For the first simulation study we choose the characteristic times to be $T = 50$ and $\tau = 100$ in order to obtain a broad spectral peak. The half power width of the peak measured in frequency bins is 33. Fig. 3 displays the results for the uniform smoothing window of different widths. Due to the symmetry of the spectrum in the neighborhood of the peak frequency, the bias ($\diamond$) between the estimated location and the true location of the peak is near to zero for small kernel widths. The standard deviation (+) is large for small widths and decreases for increasing width. The coverage probability ($\Box$) is above the nominal value of 0.9 for all smoothing widths, i.e. the confidence regions are conservative. The smallest degree of conservatism appears for a window width of $h = 5$. For the data driven choice of the kernel width, the bias is 0.2 frequency bins, the standard deviation 4.1 frequency bins and the coverage probability 0.918.

For the second simulation we choose $T = 50$ and $\tau = 500$ leading to a sharper peak of half power width 8 measured in frequency bins. Fig. 4 displays the results for the uniform smoothing window of different widths. Again, the confidence regions are conservative for all h. Because of the sharper peak, a smaller width of the smoothing window compared to the first simulation study yields the least conservative region. For the data driven choice of the kernel width, the bias is 0 and the standard deviation is 2.1 frequency bins. The coverage probability was 0.984.

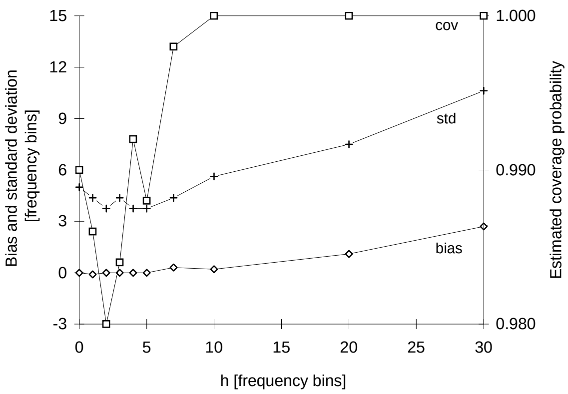

Figure 4: Result of the simulation study for an AR [2] process with $T = 50$ and $\tau = 500$. Shown is the dependence of the bias ($\diamond$), standard deviation (+) of the estimator for the peak frequency and the coverage probability ($\Box$) on the width of the smoothing window.

The Parkinsonian tremor has been shown to be a nonlinear process (Gantert et al., 1992; Timmer et al., 1993). Without claiming any physiological significance the characteristic features of this process regarding the asymmetry in the time domain and the higher harmonics in the frequency domain (see Fig. 2) can be captured by a (nonlinear) threshold autoregressive (TAR) process (Tong, 1983):

$$x(t) = \begin{cases} 1.998\, x(t-1) - 0.998\, x(t-2) - 0.03 + \epsilon(t) \\ \hfill x(t-1) > 0 \\ 1.992\, x(t-1) - 1.002\, x(t-2) - 0.2 + \epsilon(t) \\ \hfill x(t-1) \leq 0 \end{cases} \tag{13}$$

with $\epsilon(t) \sim \mathcal{N}(0, 0.1)$. Here, the true peak frequency was estimated from a spectrum that was estimated by averaging 1000 simulated periodograms. The half-power width of the main peak amounts to only 3 frequency bins reflecting the nearly deterministic behavior of tremor in Parkinson's disease. Fig. 5 displays the results for the uniform smoothing window of different widths. For the data driven choice of the kernel width, the bias is 0., the standard deviation 0.2 frequency bins and the coverage probability 0.996. The extreme conservative behavior of all estimation procedures is relativized by the fact that the average length of the confidence regions amounts to 1.2 frequency bins for the data driven estimation procedure and to 1.8 frequency bins for the fixed interval estimator with $h = 3$.

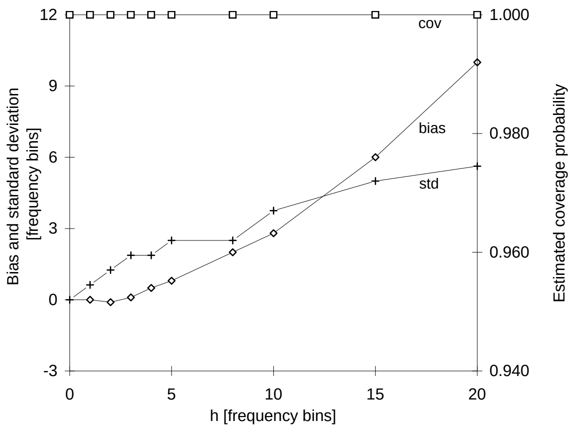

Figure 5: Result of the simulation study for a simulated Parkinsonian tremor. Shown is the dependence of the bias ($\diamond$), standard deviation (+) and the coverage probability ($\Box$) on the width of the smoothing window.

The conservatism is partially caused by the inclusion of the frequency bins where the 5 % and 95 % quantiles are located in the confidence region. Simulation studies with randomized confidence intervals reveal that these intervals are still conservative.

5 Application

We apply the proposed method to data from human hand tremor. Time series analysis methods have an increasing impact in supporting tremor diagnosis (Deuschl et al., 1996). The tremor time series are recorded by an accelerometer attached to the hand. The recording of 35 s is sampled with 300 Hz yielding 10240 data points which cover approximately 200 to 300 periods of the tremor oscillation.

Healthy subjects show a small amplitude tremor called physiological tremor. Its peak frequency ranges from 6.5 to 11.3 Hz. This range was determined from the lowest and highest peak frequency observed in 52 healthy subjects (Deuschl et al., 1996). In most cases a discrimination between physiological and pathological tremors is easy because of the different amplitudes. A differential diagnosis of the various types of pathological tremor is more difficult. The two most frequent pathological forms of tremor are the essential tremor and the tremor which might appear as a symptom in Parkinson's disease. The rate of false diagnosis between these two tremors especially in the first years of the disease is estimated to be 20 % (Findley and Koller, 1987). Essential tremor peak frequencies range from 4.6 to 10 Hz. This range was determined from 42 patients.

In Fig. 6 the spectrum of the tremor time series of a subject suffering from Parkinson's disease is displayed together with the 99% confidence region of the peak frequency for the frequency dependent choice of the smoothing width. The grey bar shows the range of peak frequencies for the healthy controls and the black bar that for patients with essential tremor. The 99% confidence region is based on 5000 resampled periodograms. The result allows for the conclusion that the considered time series was neither derived from physiological nor from essential tremor.

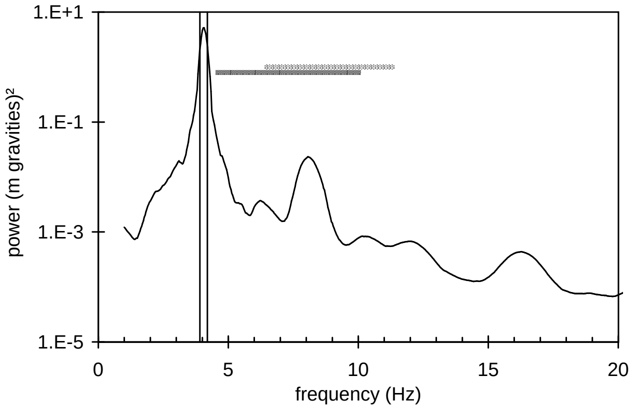

Figure 6: Estimated spectrum of a Parkinsonian tremor time series with the 99 % confidence interval for the peak frequency. The horizontal bars indicate the range of peak frequencies for healthy subjects (grey bar) and the patients with essential tremor (black bar).

For the time series of a physiological tremor displayed in Fig. 1 the estimated peak frequency was 7.30 Hz. The 95 % confidence region based on 5000 resampled periodograms was [7.04 Hz, 7.70 Hz]. The asymmetry of the confidence region reflects the slight asymmetry of the spectrum around the peak.

For the time series of a parkinsonian tremor displayed in Fig. 2 the estimated peak frequency was 5.92 Hz. The 95 % confidence region based on 5000 resampled periodograms was [5.86 Hz, 6.01 Hz]. The smaller confidence region compared to the physiological tremor reflects the sharper peak in this case.

6 Discussion

Confidence regions for spectral peak frequencies allow to describe the variability of estimators for spectral peak frequencies and, hence, contribute to the evaluation of the significance of findings.

The procedures to construct confidence regions considered in this paper depend on the smoothing width chosen to estimate the spectrum. The confidence region seems to be conservative always. Furthermore, the results of the simulation studies suggest that the data driven frequency dependent choice of the smoothing width results in a less conservative coverage probability than any fixed choice. The former method also showed a smaller bias and standard deviation of the estimator for the peak frequency than the latter.

In many other applications of the bootstrap either the data are resampled directly or new realizations are drawn from one probability density in the case of parametric bootstrap. In the case considered here, the situation is one step more complex since first the spectrum has to be estimated by smoothing the periodogram and then, for each frequency, a random variable is realized. Therefore, the resulting confidence regions depend on the chosen smoothing procedure.

The choice of an non-optimal width of the smoothing window leads to larger, i.e. more conservative confidence regions. This can be explained as follows: A smaller than optimal smoothing window causes a large variance of the spectral estimator used in the bootstrap. Consider, as an extreme example, the case of estimating the spectrum by the periodogram, i.e. no smoothing at all, see e.g. Fig. 1b. Drawing random variables according to eq. (6) and reestimating the spectra by the same, i.e. no, smoothing procedure leads to an even more erratic behavior of the reestimated spectra. Therefore, the maxima of the spectra reestimated from the realized periodograms will show a distribution which is too broad. For a broader than optimal smoothing window the peak is oversmoothed leading to an estimated spectrum which is too flat. Then, accidental fluctuations in the reestimated spectra cause a too broad distribution of the location of the reestimated spectral maxima. The optimal bandwidth minimizes these two effects. Since the smoothing window is positive definite, the peak power is always underestimated and the width of the peak is always overestimated in the finite case. This underestimation vanishes only asymptotically. Increasing number of data points for a given process leads to an increasing width of the peak measured in units of frequency bins. Therefore, the asymptotic behavior of the procedure can be judged by regarding the results of the simulation studies in reversed order than presented. This indicates a decreasing overestimation of the confidence interval with increasing number of data.

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