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Spectral analysis of a Plio-Pleistocene multispecies time series using the Mantel periodogram

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Abstract

A simple method for the spectral analysis of multispecies microfossil data through time or stratigraphic level is presented. The method is based on the Mantel correlogram, allowing any ecological similarity measure to be used. The method can therefore be applied to binary (presence-absence) data as well as raw or normalized species counts. In contrast with spectral analysis of univariate ordination scores, this approach does not explicitly discard information. The method, referred to as the Mantel periodogram, is exemplified with a data set from the literature, demonstrating several astronomically forced periodicities in microfaunal data from the Plio-Pleistocene.

Keywords: Spectral analysis; Multivariate; Astronomical forcing; Microfossils

1. Introduction

Spectral analysis of univariate time series is now commonplace in paleontology and paleoclimatology. Such analysis allows the identification of temporal periodicities due to seasonality, climatic and population dynamic cycles, or other astronomical or unknown causes. However, spectral and other time series analyses of multivariate data are not yet in common use in paleontology. Multivariate rather than univariate analysis of fossil assemblages through time takes the complete assemblage into account in an objective manner. Also, signal-to-noise ratio is likely to be improved because noise in the time series of each individual taxon will cancel out across taxa.

Multivariate spectral analysis usually follows one of two approaches. The first is multivariate extension of univariate analysis by computing a multidimensional spectrum. This spectrum is a collection of conventional univariate spectra—one for each variate but also a large number of spectra for interactions between variates. Such a multidimensional spectrum can clearly give a lot of information, but cannot be used directly for ordinal or binary data and does not give a simple overview of overall periodicity. The second approach (Jassby and Powell, 1990) is conventional univariate spectral analysis of scores resulting from of an ordination analysis such as principal components analysis (PCA), correspondence analysis (CA) or principal coordinates analysis (PCO). This involves an explicit discarding of information along all other ordination axes than the one being analyzed. PCA in particular is problematic for multispecies data where the species are likely to

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have unimodal rather than linear responses to the underlying, periodic environmental variable (Legendre and Legendre, 1998).

This paper presents a simple, intuitive spectral analysis method based on the Mantel correlogram. The analysis can utilize any multivariate similarity or distance measure, providing considerable flexibility in the type of data and the specification of similarity.

2. Methods

Univariate autocorrelation, producing a correlogram, is a basic operation in time series analysis (Roberts and Mullis, 1987). Basically, the autocorrelation sequence is a sequence of correlation values (or inner products) between the original time series and time lagged copies. For a time series $\{y(0), y(1), \ldots, y(L-1)\}$ of length L, the autocorrelation for a lag time k can be estimated by

$$\hat{r}(k) = \frac{1}{L}\sum_{l=0}^{L-1-k} y(k+l)y(l), \qquad 0 \le k < L. \tag{1}$$

Formally, the sequence is extended to negative k by $\hat{r}(k)=\hat{r}(-k)$. The autocorrelation can be normalized so that the value at lag 0 is equal to 1. Peaks in the autocorrelation function can indicate periodicities for the corresponding lag times.

Multivariate autocorrelation of a vector time series $\{\boldsymbol{y}(0), \boldsymbol{y}(1), \ldots, \boldsymbol{y}(L-1)\}$ can be defined in terms of a series of matrices, one for each lag, involving not only the correlation values for each variate (along the diagonal), but also cross-terms between variates. Disregarding the cross-terms, we can calculate an average autocorrelation sequence over all variates, as the sequence of sums of diagonal elements (the 'traces') in the series of autoregression matrices. This univariate sequence summarizes the univariate autocorrelations of all N variates:

$$\hat{R}(k) = \frac{1}{NL}\sum_{i}\sum_{l=0}^{L-1-k} y_i(k+l)y_i(l), \qquad 0 \le k < L, 1 \le i \le N. \tag{2}$$

The Mantel correlogram (Oden and Sokal, 1986; Legendre and Fortin, 1989; Legendre and Legendre, 1998; Bjørnstad and Falck, 2001) is a multivariate correlogram based on a given similarity measure. It provides a simple, univariate display summarizing the similarities between samples as a function of lag. The Mantel correlogram is usually presented in the context of spatial analysis, but is equally applicable to time series analysis. The Mantel correlogram derives its name from its historical basis in the Mantel test for association between similarity matrices (e.g. Legendre and Fortin, 1989). However, it is more clearly explained directly as a generalization of conventional autocorrelation, as follows (see also Bjørnstad and Falck, 2001). Rewrite Eq. (2) as

$$\hat{R}(k) = \frac{1}{L}\sum_{l=0}^{L-1-k} \frac{1}{N}\sum_{i} y_i(k+l)y_i(l). \tag{3}$$

This allows the equation at a specific lag k to be reinterpreted as the average of the normalized inner products of the two vectors $\boldsymbol{y}(l)$ and $\boldsymbol{y}(k+l)$, over all l. If we think of the inner product as a similarity measure between the two vectors, we can understand this value as the average similarity between samples at a temporal distance k. Clearly, we can now generalize Eq. (3) by using any similarity measure s in the place of the inner product:

$$\hat{R}(k) = \frac{1}{L}\sum_{l=0}^{L-1-k} s_{k+l,l} \tag{4}$$

This equation is in the form of a Mantel correlogram.

The power spectrum of a univariate time series can be calculated as the spectrum of its autocorrelation function. One classical method for power spectrum estimation, the Blackman-Tukey method (Roberts and Mullis, 1987), uses exactly this approach, by calculating the discrete Fourier transform of the estimated autocorrelation function. Since the autocorrelation function is symmetric around zero, the spectral coefficients will be real, as required by the power spectrum representation. The Mantel periodogram method presented here extends this idea, by considering the Mantel correlogram as an analogue to the usual univariate autocorrelation function. The Mantel periodogram is then simply the Fourier transform of the Mantel correlogram. The Mantel periodogram has been included in version 1.43 of the PAST software (Hammer et al., 2001), downloadable at http://folk.uio.no/ohammer/past.

Other methods for spectral estimation based on the univariate autocorrelation are available in the literature. One of these is the Levinson algorithm (Roberts and Mullis, 1987), which gives a spectral estimate via the coefficients of an autoregressive signal model. By increasing the order of the model (the number of terms in the linear recursion formula), the spectral resolution can be increased, at the cost of introducing spurious spectral peaks. The Signal Processing Toolbox in Matlab (The MathWorks Inc., Natick, MA) was used for the example of this method given below.