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Hunting spectro-temporal information in unevenly spaced paleoclimate time series

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Here we present some preliminary results of a statistical–computational implementation to estimate the wavelet spectrum of unevenly spaced paleoclimate time series by means of the Morlet Weighted Wavelet Z-Transform (MWWZ). A statistical significance test is performed against an ensemble of first-order auto-regressive models (AR1) by means of Monte Carlo simulations. In order to demonstrate the capabilities of this implementation, we apply it to the oxygen isotope ratio ($\delta^{18}O$) data of the GISP2 deep ice core (Greenland).

Keywords: wavelet spectral analysis, continuous wavelet transform, Morlet Weighted Wavelet Z-Transform, unvenly spaced paleoclimate time series, non-stationarity, multi-scale phenomena.

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1. Introduction

One of the main approaches used to study the climates of the past is the statistical analysis of paleoclimate time series, obtained from diverse sources (e.g. marine and lake sediments, speleothems, ice cores, etc.). Paleoclimate time series analysis is a useful mathematical tool for identifying past climate signatures archived in paleodata (Weedon, 2003; Mudelsee, 2010). However, the paleoclimatic data interpretation is not always straightforward because paleoclimate time series are generally short and noisy, do not have many elements, are usually unevenly spaced (because it is not ever possible to control the sampling intervals), may contain periodic and quasi-periodic events (in some cases, the amplitude of the periodic events registered in paleoclimate data can vary in time) or transient signals, and are a composition of numerous packages of information in scales ranging from days to millennial scales (multiscale phenomena) (Weedon, 2003; Grinsted et al., 2004; Mudelsee, 2010; Polanco-Martínez, 2012).

A powerful statistical tool for overcoming many of these drawbacks (e.g., non-stationarity, multiscale phenomena, simultaneous time–frequency analysis, etc.) is the *Wavelet Transform* (WT). The WT expands time series into the time–frequency domain and can therefore find localized intermittent signals or periodicities (Torrence & Compo, 1998; Grinsted et al., 2004). There are essentially two approaches to wavelet transforms: the first by means of the *Continuous Wavelet Transform* (CWT) and the second through the *Discrete Wavelet Transform* (DWT) (Torrence & Compo, 1998; Polanco-Martínez & Fernández-Macho, in press). The DWT is a compact representation of the data and is particularly useful for noise reduction and data compression, while the CWT is better for extracting low signal/noise ratio in time series (Torrence & Compo, 1998; Grinsted et al., 2004). As we are interested in extracting climatic signals contained in time series, in this work we focus on the CWT.

Currently, there are several statistical–computational implementations of wavelet spectral analysis techniques using the CWT (Torrence & Compo, 1998; Maraun et al., 2007; Cazelles et al., 2008). However, these tools are not able to directly handle unevenly spaced time series. A frequently used method to cope with this problem is to interpolate in time the original unevenly spaced time series in order to obtain equidistance. However, a great deal of research has shown that interpolation in time domain alters the estimated spectrum of a time series and it should be avoided (Schultz & Stattegger, 1997; Schultz & Mudelsee, 2002; Mudelsee, 2010). A more effective way to tackle this problem would be to use the *Morlet Weighted Wavelet Z-Transform* (MWWZ), which is able to directly handle unevenly spaced time series (Foster, 1996b).

The MWWZ was originally developed to analyse astronomical data (Foster, 1996b). There is an implementation of MWWZ in the literature that can be used for paleoclimate data (Witt & Schumann 2005), but it has many drawbacks. First, neither the details of this computational implementation nor the supporting software are currently available. It does not appear to include an averaging in the time and scale directions[1], and it cannot handle the bivariate case. That is, the currently available MWWZ approach lacks a statistical–computational implementation of the *Wavelet Coherence* (WCO), which is absolutely essential for the study of the relationship between unevenly spaced paleoclimate time series and environmental data.

For all these reasons, in this work we present the preliminary results of our statistical and computational implementation to estimate the *Wavelet Power Spectrum* (WPS, univariate case) by means of the Morlet Weighted Wavelet Z-Transform, which includes a statistical significance test

[1] The wavelet scalogram is a raw measurement of the time–frequency variability and could contain false spectral information (Percival & Walden, 2006). Last improvements of this technique are presented by Andronov (1998).

based on an ensemble of *first-order auto-regressive models* (AR1) following the methodology of Schulz & Mudelsee (2002) and Witt & Schumann (2005). In order to demonstrate the capability of this implementation, we apply it to a well-known unevenly spaced paleoclimate time series: the *oxygen isotope ratio* ($\delta^{18}O$) data from the GISP2 deep ice core, Greenland (Grootes & Stuiver, 1997). We have chosen this particular data set because we can compare the WPS obtained in our work with the previous results of Witt & Schumann (2005). Finally, we discuss the importance of this statistical–computational implementation for paleoclimate research.

2. Methodological and computational aspects

In this section, we describe the wavelet spectral analysis method via the Weighted Wavelet Z-transform (WWZ) and introduce an algorithm to estimate the Wavelet Power Spectrum (WPS) directly from unevenly spaced paleoclimate time series by means of the WWZ (Polanco-Martínez, 2013). In order to compute the WPS, we follow the methodology of Schulz & Mudelsee (2002) and Witt & Schumann (2005).

2.1. The continuous wavelet spectral analysis

The spectral analysis via the Continuous Wavelet Transform (CWT) is a powerful mathematical tool for studying multiscale phenomena and, more particularly, for dealing with non-stationarity (viz. the time change of statistical properties, like the mean or the variance), both commonly found in many geophysical, financial, medical, and paleoclimatic time series, among others. This tool performs a localized spectral decomposition of a time series by determining the dominant modes of variability, and how these modes change with time and scale (frequency) (Grossman & Morlet, 1984; Torrence & Compo, 1998). The CWT of a *time series* $f(t)$ with a *dilation* a and a *translation parameter* (*time shift*) τ, with respect to a *wavelet mother function* $\psi(z)$, is defined through the integral transform (Haubold, 1998)

$$W_f(a,\tau) = \frac{1}{\sqrt{a}} \int_{-\infty}^{+\infty} f(t)\, \psi^*([t-\tau]/a)\, \mathrm{d}t, \qquad a > 0 \tag{1}$$

where $\psi^*(z)$ is the complex conjugate of $\psi(z)$.

The most common wavelet function used to perform spectral analysis via CWT is the *Morlet wavelet*, which is essentially a complex exponential function with a Gaussian decay profile (Grossman & Morlet, 1984). Foster (1996b) proposed a useful simplified version of the Morlet wavelet, called the *abbreviated Morlet wavelet*

$$\psi(z) = e^{iz - cz^2} \quad \longrightarrow \quad \psi\left([t-\tau]/a\right) = \exp\left[i\,\frac{(t-\tau)}{a} - c\,\frac{(t-\tau)^2}{a^2}\right] \tag{2}$$

The constant c determines how quickly the wavelet decays. In the literature, its value is usually chosen to be $c = (8\pi^2)^{-1}$, which ensures that the exponential term decreases significantly in a single cycle $2\pi a$ (Foster, 1996b; Witt & Schumann, 2005).

The choice of a particular wavelet mother function can influence the time and scale (frequency) resolutions of the time series decomposition (Torrence & Compo, 1998; Mallat, 1999). However, the Morlet wavelet provides a good balance between the dilatation a and time localizations (Grinsted et al., 2004; Mi et al., 2005), so that it is considered one of the best mother functions in terms of reproducing the frequency decomposition of a time series (Kirby, 2005; Liu et al., 2007; Polanco et al., 2011).

2.2. The Weighted Wavelet Z-transform (WWZ)

Following Foster (1996b) and Haubold (1998), we start by proposing a straightforward, discretized version of (1), viz.

$$W_f(a,\tau) = \frac{1}{a^{1/2}} \sum_{\alpha=1}^{N} f(t_\alpha)\, \psi^*([t_\alpha - \tau]/a) \tag{3}$$

for a *time series with N data points* $f(t_\alpha)$ recorded at a discrete set of times t_α (α = 1, 2, … N). However, it turns out that, for uneven time sampling, the sum (3) is a too naive approximation to the continuous integral (1) and offers unsatisfactory performance. In order to overcome this drawback, Foster (1996b) suggested following an approach similar to that used in discrete Fourier transform (Foster, 1996a; Lomb, 1976; Scargle, 1982) by interpreting the wavelet transform (3) with Morlet wavelet (2) as a *weighted projection* onto the trial function

$$\phi(t) = e^{i\frac{(t-\tau)}{a}} \tag{4}$$

with statistical weights

$$\omega_\alpha = e^{-c\frac{(t_\alpha-\tau)^2}{a^2}} \tag{5}$$

In the theory of discrete Fourier transform, a projection determines the coefficients y_k of a set of r trial functions $\phi_k(t)$, with k = 1, 2, … r, for which the model function

$$y(t) = \sum_{k=1}^{r} y_k \phi_k(t) \tag{6}$$

fits most closely the time series under study. The best-fit coefficients y_k are determined by the formula

$$y_k = \sum_{l=1}^{r} S_{kl}^{-1} < \phi_l | f > \tag{7}$$

where $S_{kl} = < \phi_k | \phi_l >$ is the *(super-)S-matrix of the trial functions*, S_{kl}^{-1} is its inverse, and

$$< u|v > = \frac{\sum_{\alpha=1}^{N} \omega_\alpha u(t_\alpha) v(t_\alpha)}{\sum_{\beta=1}^{N} \omega_\beta} \tag{8}$$

is the inner product of two functions $u(t)$ and $v(t)$, with ω_α denoting the statistical weight assigned to the α-th data point.

Based on the above procedure, Foster (1996b) introduces the concept of weighted wavelet transform as follows. First, he replaces (4) by a set of three trial functions (r = 3) that are better suited for dealing with irregular time spacing, viz.

$$\phi_1(t) = \mathbf{1}(t) \tag{9}$$

$$\phi_2(t) = \cos\left([t-\tau]/a\right) \tag{10}$$

$$\phi_3(t) = \sin\left([t-\tau]/a\right) \tag{11}$$

He defines also the *power* for evaluating the projection statistically as

$$P = \frac{N_{\text{eff}}}{(r-1)s_\omega^2}\left[\sum_{k,l} S_{kl}^{-1} < \phi_k|f >< \phi_l|f > - < \mathbf{1}|f >^2\right] \tag{12}$$

with ϕ_k (k = 1, 2, 3) given by (9)–(11). The number $r-1$ (= 2 in this case) describes the *degrees of freedom* of the power (which is chi-squared distributed), N_{eff} is the *effective number of data points*, and $S_\omega{}^2$ is the *weighted estimated variance* of the time series. The last two are defined by Foster (1996b) as

$$N_{\text{eff}} = \frac{\left(\sum_{\alpha=1}^{N}\omega_\alpha\right)^2}{\sum_{\alpha=1}^{N}\omega_\alpha^2} \tag{13}$$

$$S_\omega^2 = \frac{N_{\text{eff}} V_f}{N_{\text{eff}}-1} \tag{14}$$

where ω_α is given by (5) and V_f, the *weighted variation of the time series* $f(t)$, is computed via

$$V_f =< f|f > - < \mathbf{1}|f >^2 \tag{15}$$

Finally, the *Weighted Wavelet Transform* (WWT) is defined by

$$\text{WWT}(a,\tau) = \frac{(N_{\text{eff}}-1)V_y}{2V_f} \tag{16}$$

where V_y, the *weighted variation of the model function* $y(t)$, is calculated in a similar fashion as (15) through the expression

$$V_y = < y|y > - < \mathbf{1}|y >^2 \tag{17}$$

For fixed scale factor a and time shift τ, the WWT can be treated as a chi-square statistic with two degrees of freedom and expected value of one (Foster, 1996b; Haubold, 1998). It turns out, however, that the WWT in (16) still has a serious shortcoming: it is very sensitive to the effective number of data N_{eff}, which leads to a shift of the WWT peaks to lower frequencies (at lower frequencies the window is wider, so that more data points can be sampled and N_{eff} becomes larger). To compensate for this fact, Foster (1996b) introduced an improved version of the WWT (16), which is less sensitive to the effective number of data, called the the *Weighted Wavelet Z-Transform*

$$\text{WWZ}(a, \tau) = \frac{(N_{\text{eff}} - 3)V_y}{2(V_f - V_y)} \tag{18}$$

As remarked by Haubold (1998), the statistical behaviour of the WWZ (18) is derived for a projection where the statistical weights are inversely proportional to the variance of the data.

In practice, the WWZ is an excellent locator of the signal frequency, but it is not a suitable measure of amplitude. Fortunately, with a projection it is easy to define the amplitude of the corresponding periodic fluctuation as the square root of the sum of the squares of the expansion coefficients for the sine and cosine functions (cf. Eqs. 6, 7, 10 and 11), which Foster (1996b) calls the *Weighted Wavelet Amplitude*

$$\text{WWA}(a, \tau) = \sqrt{y_2^2 + y_3^2} \tag{19}$$

Similarly, the wavelet phase can be computed by

$$\phi(a, \tau) = \arctan\left(\frac{y_2^2}{y_3^2}\right) \tag{20}$$

2.3. Numerical procedure to compute the wavelet spectrum

In this section we present a numerical procedure to estimate the *Wavelet Power Spectrum* (WPS) of unevenly spaced paleoclimate time series considering a red noise background. In this pilot study we use just the WWA (19) to estimate the WPS. We do not apply an averaging operator or the WOSA (Welch Overlapped Segment Averaging) procedure to smooth the wavelet spectrum. For this reason, we should be cautious with the estimation of the wavelet spectrum because this could contain false spectral information.

The statistical significance of the wavelet spectral points was tested against a red-noise process using a *first-order autoregressive model* (AR1). We have used this model because, firstly, it is known that the spectra of paleoclimatic time series show a red-noise background, that is, a continuous decrease of spectral amplitude with increasing frequency (Mann & Lees, 1996; Schultz & Mudelsee, 2002). Secondly, in the seminal work by Hasselmann (1976) it was shown that the AR1 model is enough to characterize this climatic red-noise background (an interesting explanation can be found in Mudelsee, 2010).

In order to achieve this aim, we follow the REDFIT methodology introduced by Schulz & Mudelsee (2002), which computes the red-noise Fourier spectrum of unevenly spaced paleoclimate time series based on the Lomb–Scargle Fourier Transform (also called Lomb–Scargle periodogram; Lomb, 1976; Scargle, 1982, 1989). The procedure is described as follows:

1. *Input:* $f(t_\alpha)$, the unevenly spaced paleoclimate time series under study (with the mean and linear trend removed).
2. Define some key parameters:
   a) $c = (8\pi^2)^{-1}$, cf. (2);
   b) the frequency range, defined by the minimum (lofreq) and maximum (hifreq) frequencies;
   c) the distance δfreq between successive frequencies;
   d) the persistence coefficient T_f of $f(t_\alpha)$, computed using the TAUEST program (Mudelsee, 2002).
3. Compute the WWA of $f(t_\alpha)$. For doing this, we used a program from the American Association of Variable Star Observers (AAVSO), available at the AAVSO website http://www.aavso.org/software-directory.
4. Perform a loop of Monte Carlo simulations consisting of at least $N_{\text{sim}} = 2000$ simulations:
   a) generate N_{sim} unevenly time series AR1(t_α) by using the sampling times t_α and the estimated persistence coefficient T_f (Mudelsee, 2002);
   b) compute the WWA of each synthetic AR1(t_α) time series: WWA[AR1(t_α)].
5. Compute the 95th percentile of the ensemble: WWA[AR1(t_α); $\alpha = 1; N_{\text{sim}}$]
6. Determine whether every spectral point of WWA[$f(t_\alpha)$] is significantly different from zero statistically (to the 95% confidence level), by comparing it with the 95th percentile of the ensemble.
7. *Output:* The wavelet power spectrum (WPS) with its significant spectral points.

The fact that geophysical time series have a finite length implies that discontinuities at data boundaries generally distort the wavelet power spectrum in terminal regions, which define a frequency-dependent *cone of influence* (COI). Within the COI the statistical significance of the wavelet spectral points is unreliable. Therefore, the COI imposes a serious limitation in wavelet analysis of time series that must be taken into account. There are many ways of fitting a COI into the WPS (e.g. Meyers et al., 1993; Torrence & Compo, 1998; Zhang & Moore, 2011). In this work we have padded the beginning and end of the time series under study with white noise $N(0,1)$, and then the WPS was computed. After that, we have removed the corresponding beginning and end of the WPS that were added.

This algorithm to estimate the wavelet power spectrum via the MWWZ has been programmed in the R language (R Development Core Team, 2011) and it currently runs only under Linux. A new version is now in preparation as an R package to be used on the main operative systems.

3. Case study: δ^{18}O record from GISP2

The δ^{18}O record from GISP2 is a well-known unevenly spaced paleoclimate time series, which allows us to corroborate the reliability of our statistical-computational implementation and also to compare our results with those by Witt & Schumann (2005). The record was obtained from the National Climatic Data Center, NOAA[23] and it covers the last 50,000 years (Fig. 1). It shows strong variability (with a standard deviation of 2.48), with values oscillating between −43.05‰ and −33.41‰ and a mean value of −36.44‰. Moreover, one of the most remarkable characteristics of this time series is the part that covers the last 10,000 years (covering the major part of the Holocene), which seems to reflect a bi-modal distribution (Fig. 2) and a non-stationary behaviour. Fortunately, wavelet spectral analysis is able to tackle both stationary and non-stationary time series.

On the other hand, due to the fact that the GISP2 δ^{18}O record is an unevenly spaced time series, the distance among elements is not regular: they can take values from 4.74 to 174 years, with a mean of 41.98 years. Figure 3 shows a bimodal distribution, which can be explained by different sampling rates or temporal resolutions. There are more samples and much better temporal resolution in the Holocene (last 10,000 years) than in the time period 20,000–50,000 years B.P. These sampling and statistical conditions are a challenge for the computation of the wavelet power spectrum via the MWWZ, as it will become clear in the following lines (one of the advantages of this statistical method is that it makes no use of a mean value of the distance among time samplings; rather, it needs just the lowest and highest frequencies, and an "arbitrary" constant resolution among frequencies).

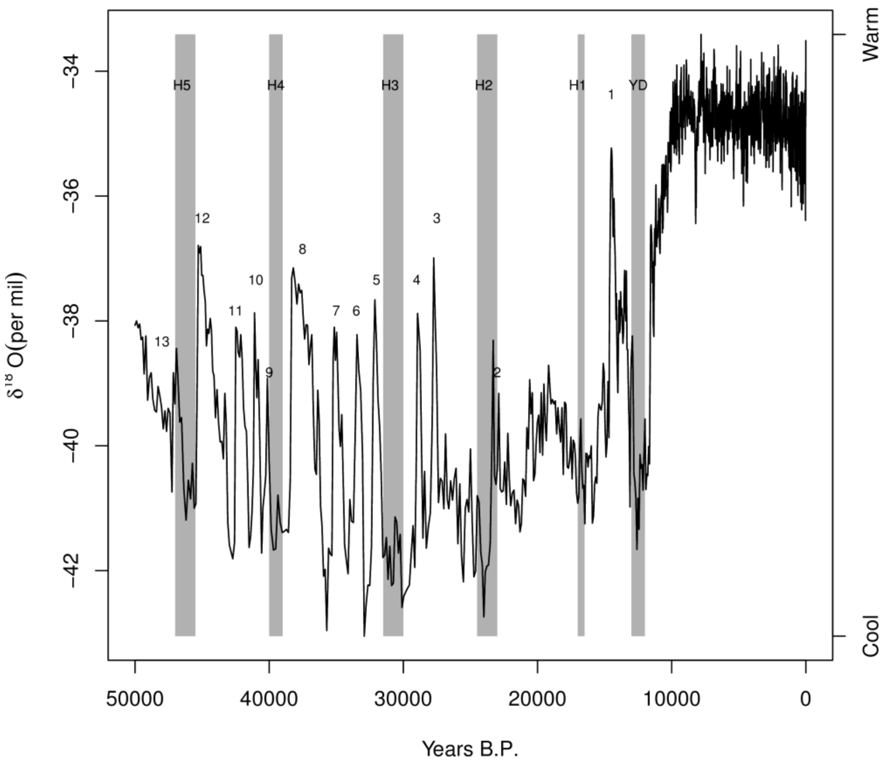

Figure 1: Time series of the GISP2 δ^{18}O (‰) record with 1,192 elements. The grey vertical bars highlight the last five Heinrich events (H1–H5) and the Younger Dryas (YD). The small numbers from 1 to 13 over certain peaks are Dansgaard–Oeschger (DO) events. The labels "warm" and "cool" at the right side indicate the range of past climates.

[2] ftp://ftp.ncdc.noaa.gov/pub/data/paleo/icecore/greenland/summit/gisp2/isotopes/gispd18o.txt

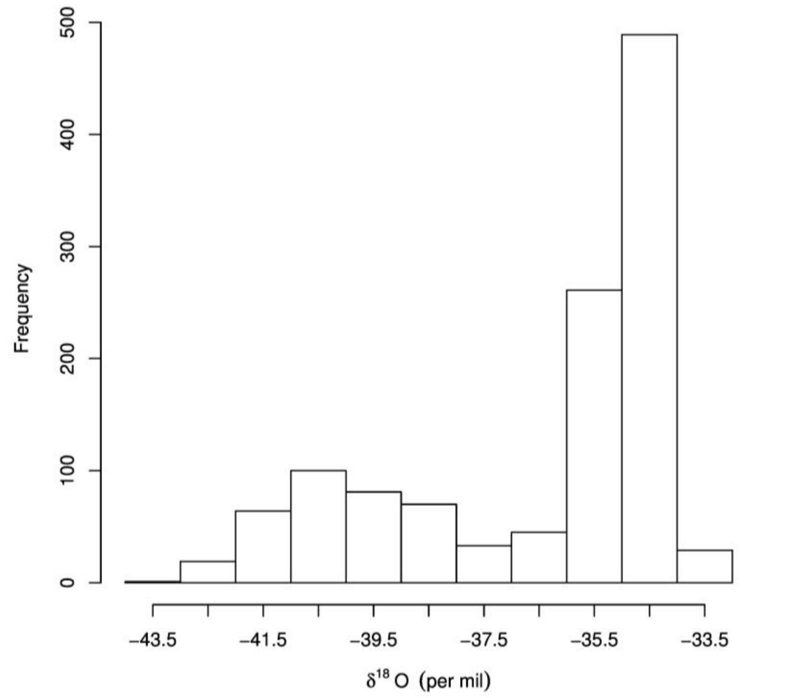

Figure 2: Histogram of the GISP2 δ18O (‰) record.

Figure 4 shows the wavelet power spectrum (WPS, not smoothed) via the MWWZ of the GISP2 δ^{18}O record. The inputs to the program are presented in Table 1). The first remarkable result is that the statistical-computational implementation to estimate the wavelet spectrum is able to detect the prominent 1,470 year spectral peak centred within the 35,000–31,000 years B.P. time interval (note that the Fourier spectral analysis is not able to provide the time intervals for the spectral peaks), a

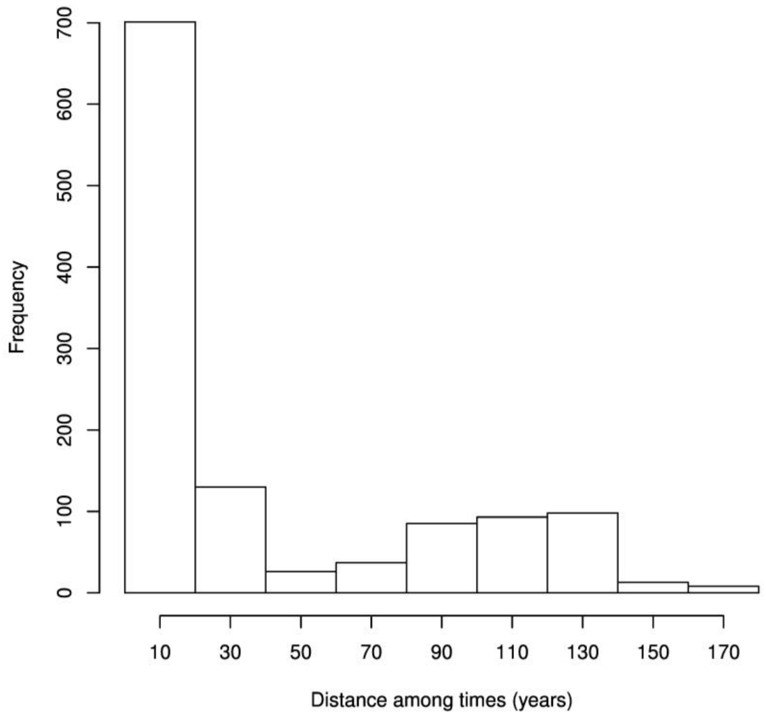

Figure 3: Histogram of the distances between sampling times in the GISP2 δ18O (‰) record time series.

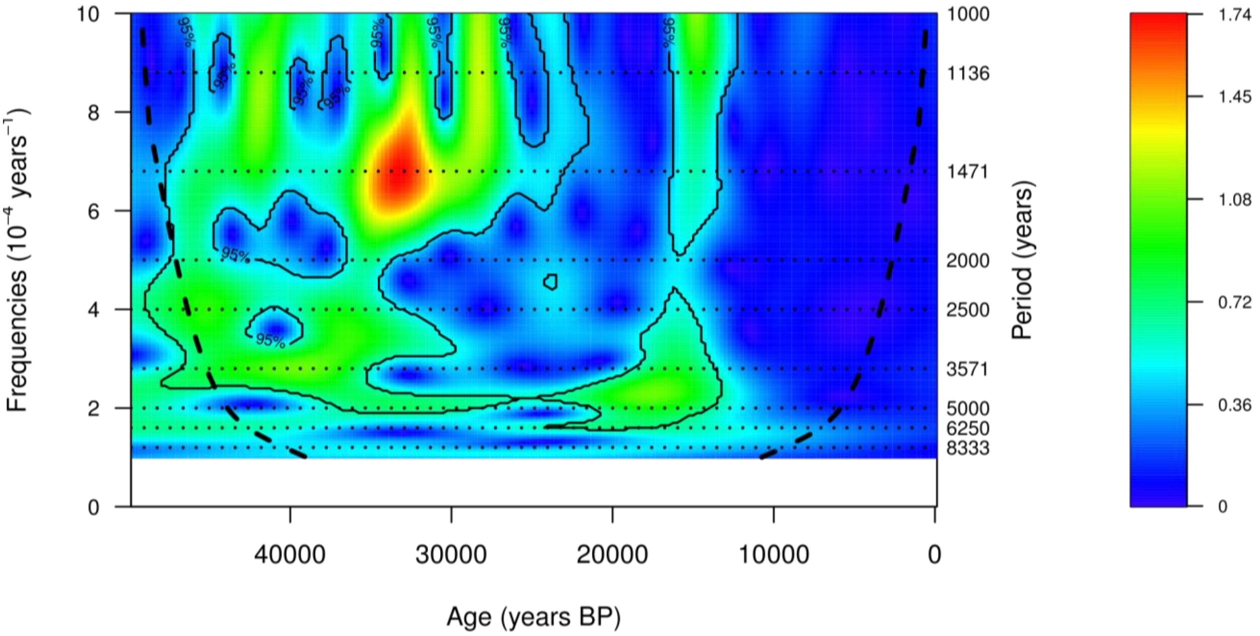

Figure 4: Wavelet power spectrum (WPS, not smoothed) of the GISP2 δ18O (‰) record, computed via the Morlet Weighted Wavelet Z-Transform (MWWZ). Contour lines indicate wavelet amplitudes that are significantly (95% confidence level) above the red-noise background. The black dashed line draws the cone of influence (COI) that delimits the region not influenced by the edge effects. The vertical box at the right side indicates the colour code of the spectral amplitudes (not normalized values) of the MWWZ.

well-known spectral signature of the GISP2 ice core record (Grootes & Stuiver, 1997). This spectral signature was also obtained by Witt & Schumann (2005) using a similar technique. There are other time intervals where the 1,470 year cycle is statistically significant, but its spectral power is not as strong as in this time interval.

Another interesting result is a couple of notorious spectral structures statistically significant located at different frequency bands and time intervals. The first is located in the time interval 48,000–28,000 years B.P. within a period range between 2,000 and 5,000 years, while the second lies in the time interval 24,000–14,000 years B.P. within a period range between 6,250 and 2,500 years. These spectral structures are far from being identical, although they share some similarities with the corresponding spectral areas found by Witt & Schumann (2005).

The conspicuous differences obtained with our statistical-computational implementation, in comparison to Witt & Schumann (2005), can be explained fundamentally by three factors: (1) the way the AR1 model was fitted (to take the red noise background into account), (2) the lack of a window smoother (either to the time or scale domain), and mainly (3) the existence of an inherent bias in the estimation of the wavelet spectrum (Liu et al., 2007). This kind of bias is also present in any kind of estimation of the wavelet spectrum by means of the continuous wavelet transform, and it is due to the fact that the wavelet transform does not produce a spectrum with identical spectral amplitudes for

Table 1: The input parameters of the program to compute the WPS via MWWZ of the GISP2 $\delta^{18}O$ record (Fig. 4). The labels lofreq and hifreq indicate the minimum and maximum frequencies of the WPS. The parameter δfreq defines the distance between frequencies, c is the decay constant of the abbreviated Morlet wavelet (2), T_f is the persistence coefficient (Mudelsee, 2002) and N_{sim} is the number of Monte-Carlo simulations (cf. Sec. 2.3).

lofreq (years^{-1})	hifreq (years^{-1})	δfreq (years^{-1})	c	T_f (years)	N_{sim}
10^{-4}	10^{-3}	5×10^{-6}	$(8\pi^2)^{-1}$	3,680	2,000

each frequency or signal. Therefore, it is required a wavelet spectrum bias correction (Liu et al., 2007). In the case of the estimation of the WPS via MWWZ, Andronov (1998) tackled this inconvenience by introducing additional weighting factors in the estimation of the wavelet spectral amplitudes. However, this task is outside of the scope of this working paper and it will be added to the next version of our statistical-computational software.

The former result and probably the most intriguing is that our statistical-computational implementation was not able to found any spectral structure statistically significant in the time interval corresponding to the Holocene (last 10,000 years). This result is not in concordance with Witt & Schumann (2005), who found red noise as well as centennial and millennial scale variability for some time intervals. A possible explanation could be due to the bi-modality of the δ^{18}O time series. However, Witt & Schumann (2005) analysed the same time series and time interval. Thus, this is probably not the cause. A more probable explanation could be related directly with the estimation of the spectral amplitudes and the statistical significance test, but further research is needed to solve this question.

4. Conclusion and future work

The statistical-computational implementation to estimate the wavelet power spectrum via the MWWZ presented in this working paper has been able to detect the main spectral signature of the unevenly spaced time series of the GISP2 δ^{18}O record, viz. the well-known spectral peak around 1,470 years. However, despite this encouraging result, our estimation of the WPS of the GISP2 δ^{18}O record is still not in full concordance with the WPS previously estimated by Witt & Schumann (2005). This means that our current implementation needs some improvements mainly related with the implementation of a window smoothing at the time or scale domain to obtain a smoothed wavelet spectrum, as well as the introduction of extra weighting factors in the estimation of the wavelet spectral amplitudes via the MWWZ (Andronov, 1998). Once these improvements are carried out, we will include the whole statistical-computational implementation into an R package to be archived in the Comprehensive R Archive Network (CRAN), in order to make this implementation freely available for the paleoclimate community around the world.

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