Estimating uncertainty in pooled proxy time-series, including stable isotopes in tree-rings

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Abstract (198 words)

Stable carbon isotope time-series ($\delta^{13}C$) from tree-rings are capable of providing valuable palaeoclimatic information, but analysis of individual tree-rings is time consuming and expensive. Pooling material from several tree-rings prior to isotopic analysis reduces costs, but does not allow the magnitude of uncertainty in the mean $\delta^{13}C$ chronology to be calculated unless the pool is broken and each tree-ring measured individually at regular intervals. Here we use a comparison of pooled and mean individual (the arithmetic mean of isotopic data from tree series measured individually) $\delta^{13}C$ records to determine whether the true error structure of the time series is better captured by using the overall mean error estimate for the entire time series or by linear interpolation between the equally spaced measurements. We conclude that where autocorrelation exists within the error structure of a chronology, annual estimates of 95% confidence intervals, developed through linear interpolation at 5-year or 10-year intervals, are preferable to using the overall mean uncertainty. The method outlined increases the viability of pooled $\delta^{13}C$ records for palaeoclimatic research by retaining error structure whilst reducing analytical time and costs. The method is applied here using tree-ring data, but could theoretically be applied to any well-replicated time-series.

Keywords: tree rings; climate reconstruction; stable isotopes; pooling; proxy time-series; error

1. Introduction

The stable carbon isotope composition ($\delta^{13}C$) of tree-ring cellulose has been used to produce valuable palaeoclimate reconstructions from many trees species, growing within a range of climatic regimes (McCarroll and Pawellek, 2001; Masson-Delmotte et al., 2005; Poussart and Schrag, 2005; Kirdyanov et al., 2008; Kress et al., 2010; Gagen et al., 2011; McCarroll et al., 2011; Seftigen et al. In press). The construction of well-replicated, multi-centennial chronologies through the analysis of individual tree-rings (Gagen et al., 2007; Young et al., 2010) permits annual assessment of isotopic variability, allowing confidence intervals to be placed around the mean isotope value and the resulting climate reconstructions (McCarroll and Pawellek, 1998; McCarroll and Loader, 2004, 2006). This method also allows identification and reduction of non-climatic trends in individual time-series (Loader et al. 2007), such as juvenile effects (Gagen et al. 2008) and physiological responses to increasing atmospheric CO_2 concentrations (Gagen et al., 2007, 2011).

The construction of long stable isotope chronologies comprising individual tree series is, however, time consuming and relatively expensive. Researchers have attempted to overcome these limitations by pooling (combining) the material from sampled trees for each year prior to isotopic analysis. Pooling of raw wood, prior to the isolation of α-cellulose, is the most commonly adopted approach, leading to a large reduction in the number of samples that have to be prepared, and this method has been successfully employed to extract climatic information from tree-rings (Rebetez et al., 2003; Treydte et al., 2007; Loader et al., 2008; Tardif et al., 2008; Hilasvuori et al., 2009; Rinne et al. 2010). Although the same weighting of each constituent tree is only guaranteed by pooling of equal amounts of well homogenised (powdered) raw wood, it has been reported that the bias from differing mass contributions of raw wood towards a pool appears to be negligible (Borella et al., 1998; Leavitt, 2008).

Pooled $\delta^{13}C$ chronologies can also be constructed by isolating the α-cellulose from individual tree-rings and creating an annual pool using equal masses from each constituent tree. Whilst this approach results in increased sample preparation time, it requires the same number of isotopic analyses as the methods outlined above and permits retention of sample material from individual tree-rings if desired. Combination of equal masses of isotopically homogenous α-cellulose ensured an equal weighting of each tree within the chronology. This method of pooling should, therefore, produce a mean isotope chronology equivalent to that obtained by calculating the mean $\delta^{13}C$ of individual trees within a chronology and is the approach adopted in this study.

A major limitation of pooled chronologies is the inability to calculate the standard deviation between the constituent trees and therefore, to assign confidence limits around $\delta^{13}C$ values. Quantification of uncertainty is an essential requirement for climate reconstructions (Jansen et al., 2007), particularly if data are to be used to test the veracity of climate model retrodictions (McCarroll, 2010). A potential solution to this problem may be to split the pooled chronology at regular intervals (eg: every 5th, 10th, 15th or 20th year) and to analyse each tree individually to calculate the standard deviation. This method was successfully applied to a pooled $\delta^{13}C$ chronology constructed using white spruce (*Picea glauca* (Moench) Voss) in subarctic Manitoba, Canada (Tardif et al., 2008), and allowed quantification of uncertainty (confidence intervals around the mean) for every fifth year.

Given a measure of uncertainty at regular intervals, there are two options for extrapolating those values so that they apply to the whole chronology: either apply the overall mean uncertainty to every annual value, or interpolate between the values in series-order to capture temporal changes in the error structure. This study aims to test whether interpolation provides a better estimate of the true error structure than simply using the mean.

2. Methods

Long-lived Scots pine (*Pinus sylvestris* L.) trees growing at Southern Glens (057°N; 005°W), western Highlands of Scotland, were sampled using a 10mm Haglöf increment borer. Cores from twenty one trees, growing on north-facing slopes (0-30° inclination) between 80 and 380m.a.s.l., were air dried for two weeks, sanded using progressively finer grades of abrasive paper and crossdated using a binocular microscope and Velmex measuring stage interfaced with a computer. TSAPWin^{TM} and COFECHA (Holmes, 1999; Grissino-Mayer, 2001; Rinn, 2003) were used to absolutely date each tree series and a detrended ring-width chronology for Southern Glens was constructed using the computer program ARSTAN (Holmes, 1983). Under the magnification of a binocular microscope, annual whole-ring (early- plus late-wood) increments were cut into thin slivers using a scalpel. α-cellulose was isolated from annual raw wood samples using standard techniques (Loader et al., 1997; Rinne et al., 2005). In order to produce isotopically homogenous sample material, the resulting α-cellulose was placed into 2mm micro-centrifuge tubes with deionised water and homogenised using a Hielscher UP 200S ultrasonic probe (Loader et al., 2008; Laumer et al., 2009). Following freeze drying (ModulyoD Thermo Savant), an equal quantity of alpha-cellulose (0.5mg ±0.05mg) was removed from each annual individual cellulose sample and combined to produce an annual pool. Pooled samples were then placed in deionised water and homogenised again, before being freeze dried. Between 0.30 and 0.35mg of alpha-cellulose were weighed into tin foil capsules, crimped and placed into a sample tray. Stable carbon isotope analysis was conducted on ANCA and SerCon GSL elemental analysers (1000°C combustion temperature), interfaced with 20-20 Isotope Ratio Mass Spectrometers (IRMS) (PDZ-

Europa). Stable isotope results are expressed as per mille (‰), relative to the international standard Vienna Pee Dee Belemnite (VPDB) standard (Coplen, 1995, 2006).

The $\delta^{13}C$ chronologies presented here were produced for the purpose of palaeoclimate reconstruction, so they have been corrected both for changes in the isotopic ratio of atmospheric carbon dioxide, by simple addition using (and extrapolating) the values provided by McCarroll and Loader (2004), and for changes in intrinsic water-use efficiency in response to increased atmospheric carbon dioxide (CO_2) concentration, using the Pre-INdustrial (PIN) correction proposed by McCarroll et al. (2009). Both pooled and mean individual $\delta^{13}C$ chronologies comprise a minimum of seven trees between AD 1650 and 2007. The pooled record incorporates one specimen which was omitted from the mean individual chronology. Tree 50B (AD 1715-1820) does not demonstrate a common signal with the mean individual chronology ($r = -0.10$, AD 1715-1820). This is beneficial, as it provides the opportunity to assess whether incorporation of a "noisy" series significantly affects the isotopic signal of the pooled $\delta^{13}C$ chronology at this level of replication.

Annual 95% confidence intervals were calculated for the mean individual chronology using the equation given below, where *n* is the number of trees in a given year, SD is the standard deviation of those trees, and *t* is the *t* distribution value for *n* in that year.

$$\text{95\% confidence interval} = t \cdot \left(\frac{SD}{\sqrt{n}}\right)$$

Annual confidence intervals were calculated through linear interpolation between equidistant pairs of data points (observed confidence intervals). Interpolated datasets were developed for intervals of 5, 10, 15 and 20 years and for all possible combinations of years within these categories (e.g. AD 1650, 1651….1654 for 5-year intervals). Therefore, the sensitivity of interpolation to choice of years can be assessed. The reduction of error (RE) statistic (National Research Council 2007) is used to assess whether the interpolated values have greater predictive skill than simply using the overall mean. This should permit the identification of an optimum sampling resolution, whereby the cost of interpolation remains advantageous and still retains the error structure of a time series better than the mean. The equation for RE is given below, but the terms of the equation have been adjusted for this study.

$$\mathrm{RE} = 1 - \left[\frac{\sum_{i=1}^{n} \left(x_i - \hat{x}_i \right)^2}{\sum_{i=1}^{n} \left(x_i - \bar{x}_c \right)^2} \right],$$

where x_i and $\hat{x}_i$ are the observed and interpolated 95% confidence intervals in year *i* and $\bar{x}_c$ is the mean of the observed confidence intervals for the entire time series. Years which were used in the interpolation equation were omitted prior to the calculation of RE.

3. Results

Pooled and mean individual isotope chronologies

A strong relationship (r = 0.85; P<0.01, n = 358) exists between mean individual and pooled $\delta^{13}C$ chronologies for Southern Glens from AD 1650-2007 (Figure 1). Both chronologies have very similar mean values (pooled = –24.14‰; mean individual = –24.18‰) and variances (pooled = 0.08‰; mean individual = 0.09‰) throughout this period and exhibit near identical trends at high and low frequency timescales. An *F*-test, followed by a z-test (Fowler et al., 1998), demonstrates that there are no significant differences (P = 0.05) between the variances (F = 1.09; F-critical = 1.19) or means (z = 1.77; z-critical = 1.95) of the pooled and mean individual $\delta^{13}C$ chronologies from AD 1650-2007.

Figure 1

The incorporation into the pooled chronology of a noisy series (tree 50B, AD 1715-1820) does not result in any significant difference in either variance (F = 1.29; F critical = 1.38) or mean value (z = 0.19; z critical = 1.95) between the two chronologies during this period and they remain highly correlated (r = 0.74; P<0.01).

Assessment of error structure

Normally, one would assume that the inter-annual error is independent. However in many proxy timeseries based upon biological systems this may not always be the case. The non-parametric 'number of runs test' demonstrates that the true uncertainty values, at annual resolution, are not randomly arranged through time (z = –8.54, P<0.0001, n = 358). This is confirmed by the presence of significant autocorrelation within the time series (r_1 = 0.61, P<0.01, n = 357). The error structure of the annual time series is thus far from white noise, and the uncertainty for a given year is not independent of the uncertainty for the surrounding years. This means that there is at least the potential for interpolation to capture some of the real error structure of the time series.

The value of interpolation is assessed here by using the results from the individual tree-rings to produce artificial pooled chronologies. As values are available for every tree in every year, we can therefore assess the effect of varying the interval at which the artificial pool is broken and also assess the sensitivity of the results to the individual years on which the interpolation is based.

When the pool is broken every five years, it is clear that linear interpolation follows the true error structure of the data very well (Figure 2A). Almost 74% of the interpolated values fall within 0.1‰ of the true values, compared with only 59% when the overall mean is used. The superiority of interpolation over the mean is demonstrated by a positive RE value (0.30). Splitting the pool every ten years still produces interpolated values that follow the true error structure very well, with almost 70% of interpolated values falling within 0.1‰ and a positive RE value (0.20). A 10-year interpolation interval thus provides an 11.7% increase in data that are distributed within 0.1‰ of observed values, relative to using the mean (Table 1).

As the sampling interval exceeds 10 years, more individual series fail the RE test because the coincidence of interpolation intervals with extreme values in the error structure affect a greater proportion of the dataset. Interpolation is not a “perfect” solution; this is highlighted by the 10-year interpolated series starting in AD 1656, which is influenced by a relatively extreme isotopic value. Removal of a single extremity (AD 1766) results in an increase in RE from -0.10 to 0.20. Even with a spacing of 15 years, interpolation performs better than the overall average. A reasonable guide to the likely advantage of using interpolation is provided by the first order autocorrelation of the error estimates (Table 1), since as this approaches zero there can be no advantage over using the overall average error.

Figure 2 shows examples of 5, 10, 15 and 20 year interpolated series, starting with the year AD 1650. The histograms and line graphs (A-D) confirm that interpolation is most effective when the distance between sampling intervals is equal to, or less than, 10 years. Beyond this length of interval, less of the trend in the error structure is captured.

Table 1

Figure 2

Addition of the observed, interpolated (10-year intervals starting AD 1650) and mean (10-year intervals) 95% confidence intervals to the pooled $\delta^{13}C$ chronology (Southern Glens) appear to yield very similar levels of uncertainty (Figure 3, graph C), a result of the larger variance in the $\delta^{13}C$ data (0.08‰), relative to the error time series (0.01‰). A section of the chronology presented in graphs A and B (Figure 3) demonstrate how interpolation at 10-year intervals is more capable of retaining the error structure of the chronology, relative to the mean.

Figure 3

4. Discussion and Conclusions

Prior to this study, a number of pooling methods had been proposed for stable isotope dendroclimatology (Leavitt and Long, 1984; Boettger and Friedrich, 2009), but there was a lack of knowledge regarding the relationship between pooled and mean individual chronologies and no practical approach to quantifying uncertainty. The large-scale comparison presented here confirms that equally-weighted, pooled (α-cellulose) $\delta^{13}C$ chronologies developed from Scots pine trees growing at Southern Glens are equivalent to chronologies constructed by taking the mean $\delta^{13}C$ of individual trees. Therefore, this method is presented as a viable means of constructing a pooled $\delta^{13}C$ chronology, with a significant reduction (typically 60-80%) in the number of required analyses. Pooling raw wood prior to chemical treatment to isolate α-cellulose would result in further savings.

Splitting the pool at regular intervals, and measuring the isotopic ratio of each ring individually, provides equally spaced measurements of between-tree variability and therefore of the uncertainty in the estimate of the mean. By using a well replicated $\delta^{13}C$ chronology, where every tree-ring was measured individually, we were able to simulate pooled chronologies where the position and spacing of the splitting could be varied. The error structure of the time series, at annual resolution, was far from white noise, showing significant autocorrelation. Consequently, we found that given a spacing of 5 or 10 years, linear interpolation between adjacent split pool measurements provided a better approximation to the true error structure than simply applying the overall mean uncertainty to every year.

The optimum period to split a pooled chronology is a function of the degree of autocorrelation in the error structure (not the isotope values) and will therefore vary with each data set. Appropriately replicated tree-ring stable isotope chronologies constructed using a varying numbers of trees, which enter and leave the chronology at different times, are very likely to have error structures that differ significantly from white noise and in these situations, the interpolation approach would lead to an improvement in error estimation. When a chronology is produced by pooling alone it is not possible to measure the true error structure, but our results indicate that the first order autocorrelation observed in the split pool samples (Table 1) provides a reasonable guide to the relative merits of either interpolating the errors or just using the overall mean. When a pooled sampling approach is being applied to a new site, where the error structure of the data is completely unknown, we suggest that splitting the pool every ten years and interpolating the uncertainty is a reasonable compromise between the cost of analyses and the need to quantify the uncertainty around the mean.

This research has increased the viability of pooled $\delta^{13}C$ chronologies through proposing and testing a method of estimating annual confidence intervals. Whilst this approach may not always identify individual years where confidence intervals vary significantly from adjacent years, it has been identified as an effective approach for assessing and maintaining temporal variability in uncertainty around a chronology. The method outlined significantly reduces the analytical time and expense of constructing $\delta^{13}C$ chronologies and is likely to be applicable to other stable isotope (oxygen and hydrogen) series from tree-rings or to other well-replicated proxy records.

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Figure
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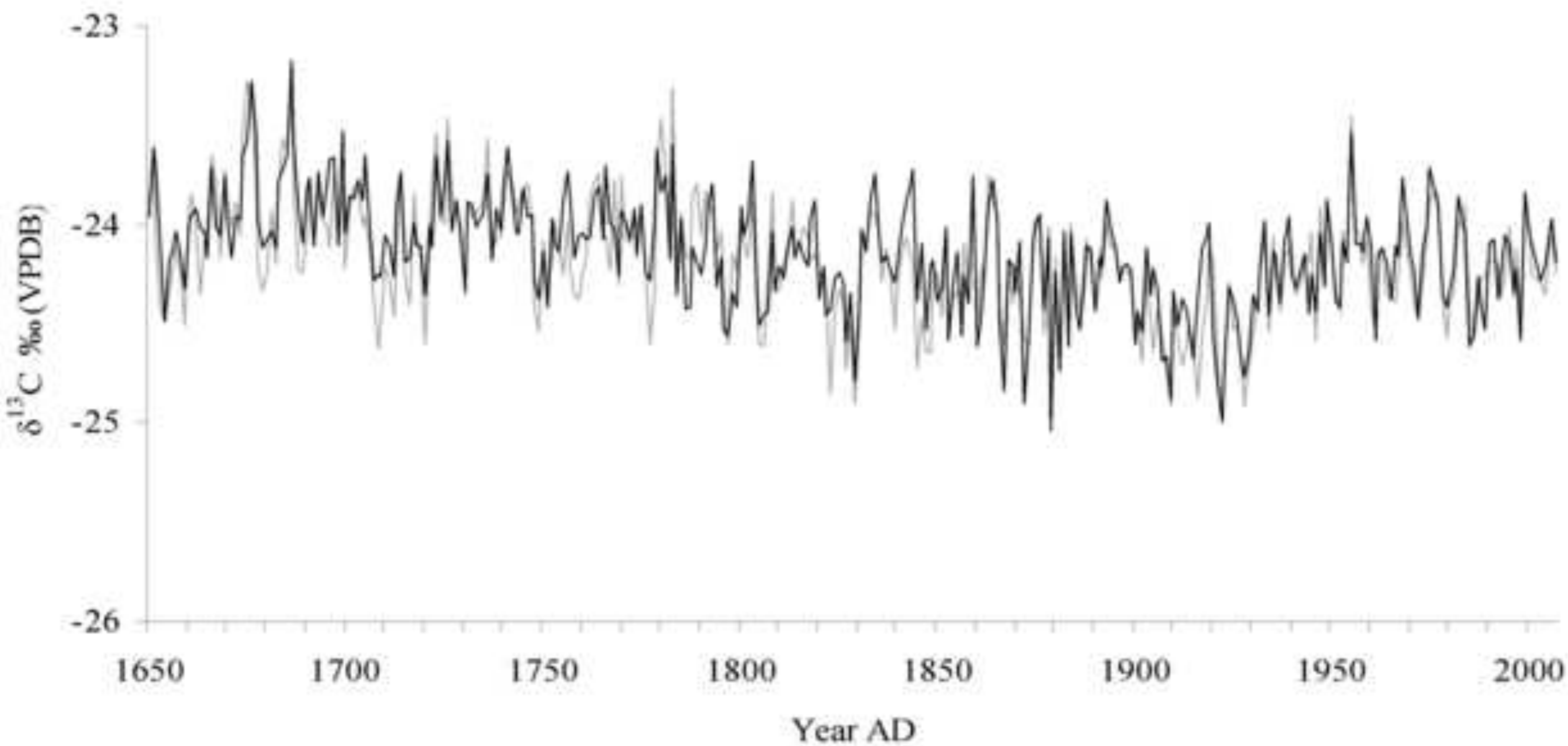

Figure 1: Comparison of pooled (black line) and mean individual (grey line) $\delta^{13}C$ chronologies for Southern Glens between AD 1650 and 2007. The two chronologies are highly correlated over this time period ($r = 0.85$, $P<0.01$, $n = 358$).

Figure
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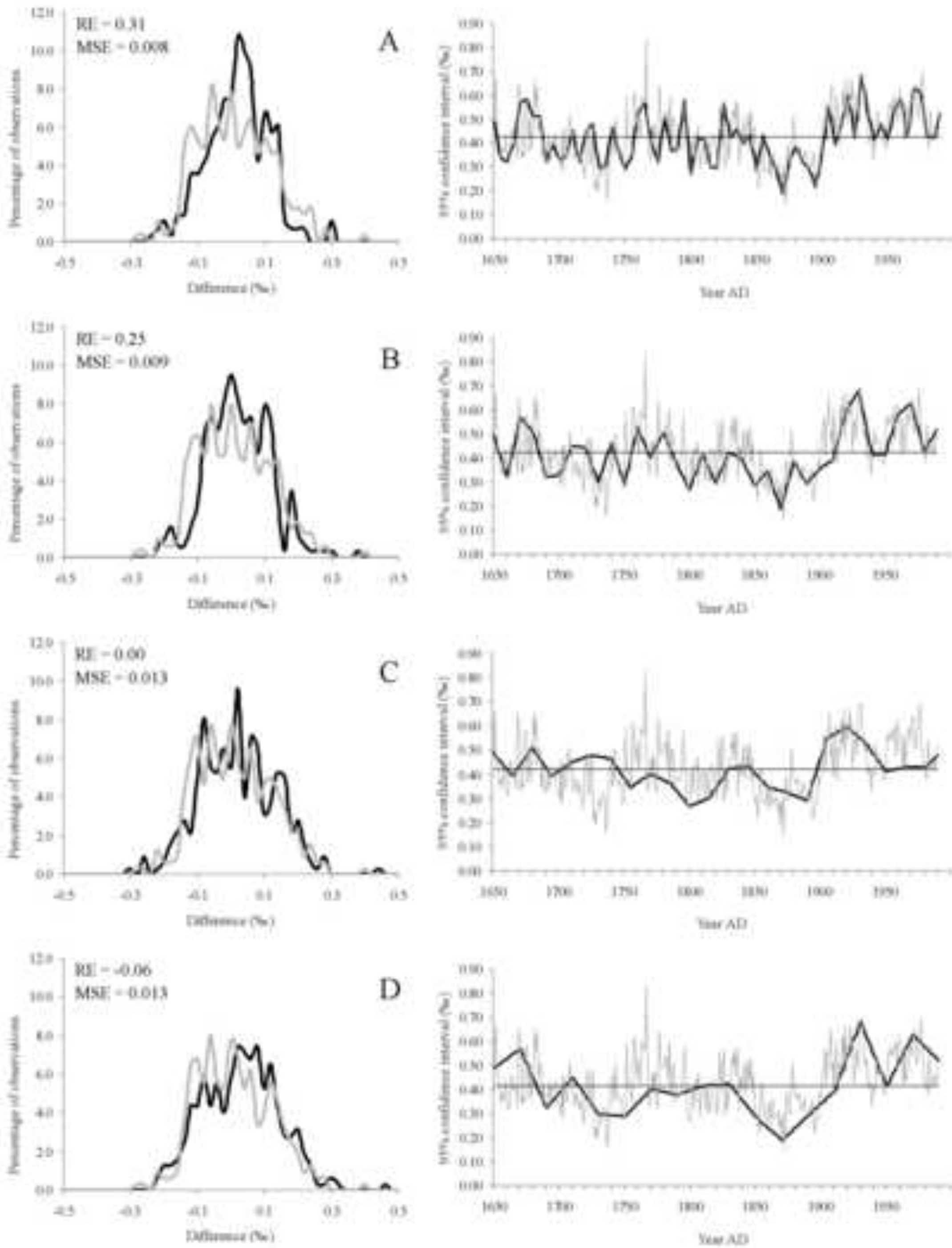

Figure 2: Histograms showing the difference (‰) between observed minus interpolated confidence intervals (black line) and observed minus mean confidence intervals (grey line). The line graphs show the observed confidence intervals (grey line) and the interpolated confidence intervals (black line) for the Southern Glens chronology. The horizontal black line represents the mean observed uncertainty for the interpolation intervals throughout the chronology. Comparisons of observed and interpolated data are presented (starting with the year AD 1650) for 5 (A), 10 (B), 15 (C) and 20-year intervals (D).

Figure
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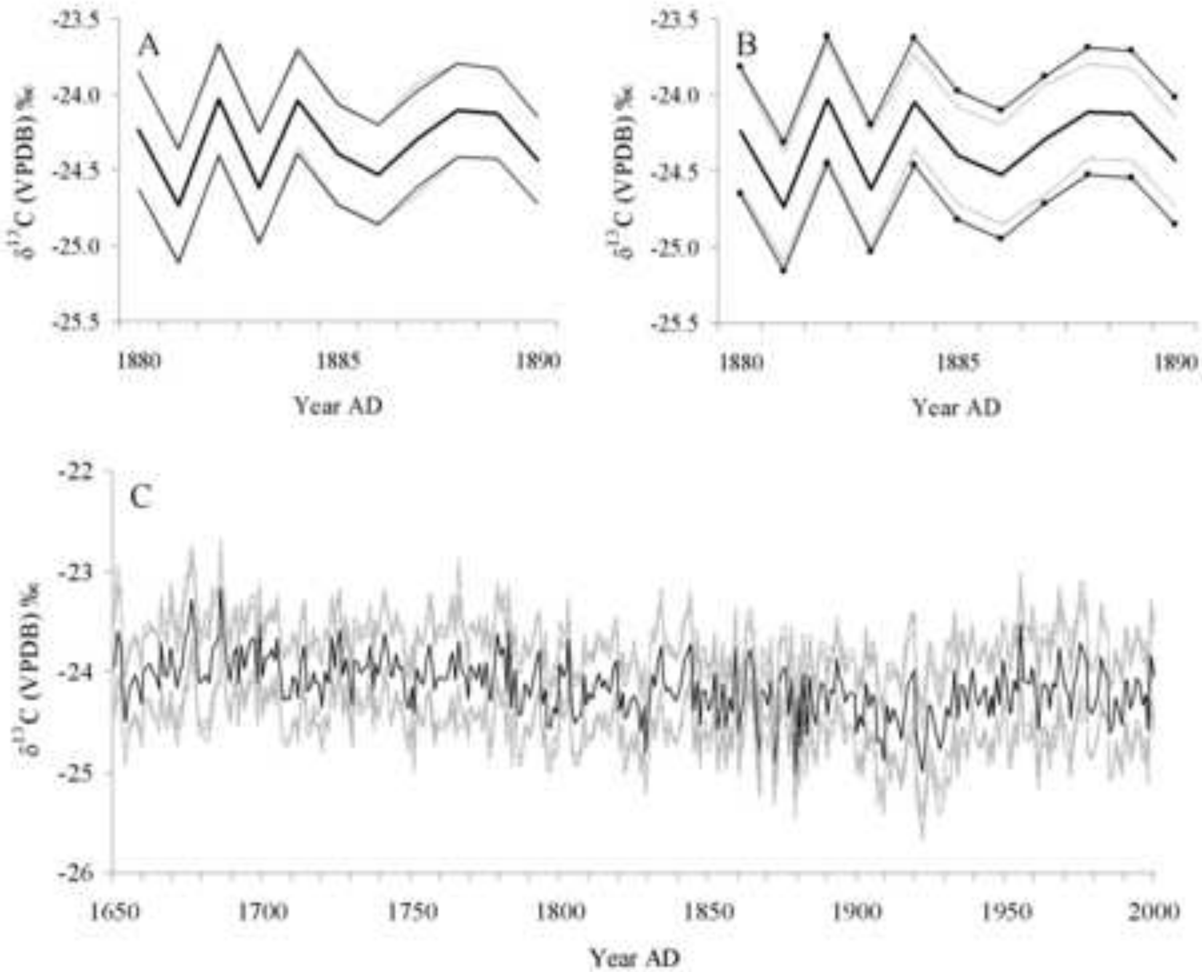

Figure 3: The addition of 95% confidence intervals to the pooled δ13C chronology (Southern Glens). The difference between observed (grey line) and interpolated (black line) (A) and observed and mean confidence intervals (black circles) (B) is shown for a short section (AD 1880-1890) of the chronology (thick black line). The differences between observed, interpolated and mean confidence intervals (grey lines) appear insignificant when applied to the pooled δ13C chronology (black line) (C), a result of higher variance in δ13C values (0.08‰) relative to the observed error structure (0.01‰) between AD 1650 and 2007.

Table 1: Comparison of mean first order autocorrelation, mean MSE, mean RE and the relationship between observed, interpolated and mean confidence intervals for 5, 10, 15 and 20-year intervals.

	Interpolation interval			
	5-years	10-years	15-years	20-years
Observed - interpolated				
Mean MSE	0.008	0.010	0.011	0.011
% of data within 0.1‰	73.7	69.9	67.3	65.8
% of data within 0.2‰	96.7	95.5	94.7	79.5
Observed - mean				
Mean MSE	0.012	0.012	0.012	0.012
% of data within 0.1‰	58.8	58.2	58.4	58.0
% of data within 0.2‰	94.1	93.9	94.0	93.9
First order autocorrelation	0.41	0.26	0.20	0.08
Mean RE	0.30	0.20	0.11	0.09