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Methods and code for ‘classical’ age-modelling of radiocarbon sequences

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ABSTRACT

Age–depth models form the backbone of most palaeoenvironmental studies. However, procedures for constructing chronologies vary between studies, they are usually not explained sufficiently, and some are inadequate for handling calibrated radiocarbon dates. An alternative method based on importance sampling through calibrated dates is proposed. Dedicated R code is presented which works with calibrated radiocarbon as well as other dates, and provides a simple, systematic, transparent, documented and customizable alternative. The code automatically produces age–depth models, enabling exploration of the impacts of different assumptions (e.g., model type, hiatuses, age offsets, outliers, and extrapolation).

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1. Introduction

Age–depth models are built to estimate the calendar ages of depths in a core from a deposit, based on limited numbers of dated depths and on assumptions as to how the deposit has accumulated between those dated depths. Given the intensive use of age–depth modelling, surprisingly few details have been published about the techniques involved, adequate software seems to be largely missing or under-used, and details of applied age–depth modelling assumptions are often missing in the literature.

A review of all papers published in 2008 in the journals Quaternary Geochronology, Quaternary Science Reviews, Journal of Quaternary Science and The Holocene, indicates 93 papers applying some kind of age–depth model through fossil proxy deposits (Table 1). Of these papers, all 82 that used $^{14}$C dates provide details about their calibration procedures (e.g., which calibration curve and software were applied). However, often much less information is supplied about subsequent age–depth modelling (regularly this information can only be gleaned from graphs). Sixty papers do not tell which (if any) point estimates were used, 71 do not mention the software used to produce age–depth curves, 65 do not indicate whether age–depth uncertainties were calculated, and 18 do not specify the applied age–depth model. Eleven papers apply some form of Bayesian age–depth modelling, whereas the remainder use “classical” age–depth modelling such as linear interpolation (31) or linear/polynomial regression (18).

As will be discussed below, calibrated $^{14}$C dates often have irregular distributions which cannot be properly reduced to single point estimates with symmetric error bars. However, most age-modelling routines do indeed simplify calibrated distributions to symmetric ones. Bennett (1994) and Bennett and Fuller (2002) discussed basic age–depth models based on linear interpolation, polynomial and spline regression, but based on uncalibrated radiocarbon dates. Proxy graphing software Tilia (Grimm, 1990) produces age–depth models, but it does not calibrate dates, it ii) does not take into account errors, and iii) does not provide age–depth graphs. Heegaard et al. (2005) applied mixed-effects modelling, but assumed that calibrated $^{14}$C ages can be approximated by a simpler statistical distribution (e.g., Gaussian). It is likely that studies which do not report their age–depth modelling software often use regression or spline functions which generally cannot deal with irregular distributions. Whereas proxy graphic software psimpoll (Bennett, 1994) can handle calibrated $^{14}$C dates, they need to be calibrated outside the software. Although Bayesian methods can produce very reliable age–depth models (e.g., Blaauw and Christen, 2005; Bronk Ramsey, 2008), Table 1 shows that by far most studies continue to use more basic, ‘classical’ age–depth models (especially for sites with only a handful of dates). Here these classical approaches will be discussed, and a technique based on probability sampling methods will be proposed in order to take into account the multi-modal and asymmetric nature of calibrated $^{14}$C dates. A more systematic and transparent approach to produce classical age–depth models is presented, based on free and open-source software.
2. Radiocarbon calibration

The importance of using calibrated $^{14}$C dates cannot be overstated. Owing to past changes in atmospheric $^{14}$C concentration, the relationship between $^{14}$C and calendar age is far from linear, thus requiring a calibration curve (Reimer et al., 2009). Whereas an uncalibrated $^{14}$C date can be assumed to have symmetrical errors (normal distribution), calibration will often result in widened, asymmetrical and multi-peaked calendar age uncertainties (Fig. 1; all distributions are of arbitrary heights. From left to right, white crosses indicate the date’s midpoint, weighted mean, median and mode, respectively. Multiple calendar ages intercept $2450 \pm 30 \, ^{14}$C BP at 2 standard deviation. Highest posterior density ranges (dark grey) are $2359–2546$ (probability 57.6%), $2560–2574$ (2.5%), $2578–2616$ (10.6%) and $2635–2701$ cal BP (24.7%). Axes of the probability range, taking into account their asymmetric and multi-peaked shapes. In standard calibration software such as CALIB (Stuiver et al., 2005), these ranges are obtained by calculating the highest posterior density (hpd) ranges: i) probability distributions are normalised to 100% (Eq. (1)), ii) the calendar years are ranked according to their probabilities, iii) those calendar ages with a cumulative summed probability at or below the 1 sd (c. 68%) or 2 sd (c. 95%) threshold are retained, and iv) the extremes and probabilities of any sub-ranges within these calendar ages are found (Fig. 1).

The probabilities within hpd ranges are either reported as ratios of the entire calibrated distribution (where the hpd ranges add up to say 68% or 95%; OxCal, Bronk Ramsey, 2008), or as ratios of the hpd region only (where the ranges are normalised to 100%, e.g., CALIB, Stuiver et al., 2005). Calibrated ranges at 1 sd will obviously result in narrower confidence intervals, and thus a perceived higher precision, than at 2 sd. However, given the often asymmetric and multi-modal nature of calibrated distributions, the probability that the ‘true’ calendar date lies outside the 1 sd ranges is considerable (c. 32%). Therefore the use of non-normalised 2 sd calibrated ranges is preferable.

Non-$^{14}$C dating information, such as a tephra layer of known or estimated calendar age, a historically anchoring pollen event, or a modern age for the top of a sequence (e.g., the year of sampling), can provide additional dating points for age-depth modelling. Whenever available, it is advisable to include such data, with an estimate of their chronological uncertainty.

\[ y \sim N(\mu(\theta), \sigma^2) \]
3. Age–depth modelling

Having estimated the age distributions of the individual dated depths, the next step is to provide age estimates for all depths in a sequence. This is done by modelling the accumulation of the sequence through time. The researcher will have to decide on the most likely type of age–depth model. For example, a deposit in a stable environment will probably have accumulated with fewer events of hiatuses or accumulation rate changes than one from a more variable environment, and should thus probably be modelled using a smooth age–depth model. The very common age–depth model of linear interpolation between the dated levels (Table 1), assumes that abrupt changes in accumulation rate took place exactly at the dated depths. Although this assumption is often likely to be wrong, linear interpolation often produces what look like plausible age–depth models (Bennett, 1994). In some sequences one or more hiatuses appear present, requiring models through subsets of the data. Additionally, at times age–depth models need to be extrapolated beyond the dated levels (necessarily introducing a large degree of age–model uncertainty for the undated parts of the sequence).

Calibrated distributions and ranges of 14C dates, and resulting uncertainties in age–depth models, often span several centuries. Even so, users often require a single ‘best’ age–depth model in order to plot proxy values against calendar age. Drawing straight, polynomial, or exponential curves through age–depth data with symmetrical errors is straightforward and can be done automatically in spreadsheets and age-modelling software such as psimoll (Bennett, 2008), the age–depth code of Heegaard et al. (2005), and Tilia (Grimm, 1990). Similarly, confidence intervals of such interpolation or regression curves can be easily calculated using standard techniques.

However, 14C ages are notorious for their highly asymmetric calibrated distributions, and reducing them to single points is problematic (Telford et al., 2004b; Michczyński, 2007). To take the date of Fig. 1 as example, its midpoint of the 95% hdq ranges lies at 2530 cal BP, a year with rather low calibrated probability. Also other point estimates such as the median (2508 cal BP) or the weighted mean (2528 cal BP) fall at unlikely calendar ages. The year with the highest probability (mode or intercept; 2486 cal BP) is an inadvisable point estimate, owing to (i) the possibility of multiple intersecting calendar years and (ii) its sensitivity to small variations in the calibration curve (Telford et al., 2004b). Moreover, the error ranges of all these point estimates (except the midpoint) will often be asymmetric. Therefore classical statistical regression techniques which depend on symmetric error distributions should not be applied to 14C age–depth modelling.

A proposed alternative to the above point estimates is to use the entire calibrated distribution of the dates. This can be done by repeated random sampling of the calibrated distributions of the dates, each time calculating an age–depth model through the sampled ages. If a large number of calendar ages is drawn from a calibrated distribution \( f(d) \), with the probability of an age being sampled proportional to its height of the probability distribution at that age (see Eq. (1)), a histogram of these age estimates will form a close approximation of the original calibrated distribution (Fig. 2). This technique is known as importance, bootstrap or Monte Carlo sampling; Bayesian age–depth modelling makes use of comparable though more sophisticated iterative sampling methods.

Similar to estimating calibrated distributions by importance sampling, for a core with multiple dates we can sample ages from each of its calibrated distributions \( f(d|\theta) \) for each of \( n \) dated depths), thus resulting in point age estimates for all dated depths (Fig. 3). A curve can then be drawn through these age–depth point estimates, resulting in a calendar age estimate for any depth \( d \) (dated or undated). Repeated sampling and subsequent age–depth modelling will thus result in multiple age estimates for depth \( d \), and histograms from a sufficiently large amount of iterations will provide us with a calendar age distribution of this depth, \( f(d|\theta) \). The explicit assumption made here is that although the true calendar ages of a core’s dated depths will never be known, the type of age–depth curve applied through these unknown points (e.g., a smooth spline) will be a reliable approximation of the unknown true accumulation history of the site. Through repeated sampling of the calibrated distributions, each time calculating its age–depth model, we will thus build up an approximation of the site’s accumulation history, based on the dated depths, their uncertainties, and a chosen type of age-model. This procedure can be run in psimoll (Bennett, 2008) by feeding it age distributions calculated by, e.g., BCal (Buck et al., 1999) for an application see Velloff et al. (2006). A comparable bootstrap procedure was reported by Higuera et al. (2009).

Heegaard et al. (2005) using mixed-effect modelling to add an extra error term to dated levels, with the aim to include an

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Fig. 2. Two thousand point calendar year estimates (short lines at bottom graph) were sampled from the calibrated distribution of the date of Fig. 1 (dark grey distribution). As explained in the text, calendar years with higher probabilities were sampled more frequently. A histogram of the sampled ages (light grey bars) closely resembles the original calibrated distribution.

Fig. 3. Schematic drawing of an iterative sampling process in age–depth modelling. Four point estimates (coloured crosses) are sampled from calibrated distributions (grey histograms), and error-weighted smooth splines drawn through the crosses (each colour corresponds to an iteration process). Note that the splines do not necessarily cross each individual age point estimate. Splines were weighted by the calibrated probabilities of the sampled calendar ages. The grey envelope shows the final 95% confidence intervals based on 1000 iterations. The age distribution of all splines at 200 cm depth is indicated by the blue histogram. The shown data are a selection from core Quillichao (Bertino et al., 2002; Fig. 4). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)
uncertainty as to whether the reported date of a dated level is a true representation of its real age (e.g., see Scott, 2007 for the variability between repeated 14C measurements on a single piece of wood). However, Heegaard et al. (2005) did not use calibrated distributions and instead assumed that these can be approximated by symmetrical distributions. For calibrated distributions, the “Heegaard” added error could be simulated by sampling say 1000 14C ages from a reported 14C age (y ± sd), assuming a normal distribution for the 14C measurement. Then each sampled 14C age is calibrated, and a single calendar year is sampled from its calibrated distribution (Eq. (1)). As with the sampling method described above, a histogram of the mixed-effect sampled calendar ages will form an estimate of the date’s calibrated distribution. As expected, mixed-effect age-models generally obtain wider confidence limits than models without the added error (data not shown).

Even if all uncertainties have been taken into account, users often need a single ‘best’ age–depth model in order to produce plots of the core’s analysed proxies against age (however, see Blaauw et al., 2007 for plots which include chronological uncertainties of proxies). As explained above, there are considerable problems with age-depth models through point estimates based on the midpoints, (weighted) mean, median or mode of calibrated dates. Even more, the considerable scatter between closely spaced dates, as well as between dates and the applied model, indicates that the accuracy of 14C measurements should not be overestimated (see Scott, 2007 for the variable outcome of repeated 14C dating of a single sample). As an alternative to drawing ‘best’ age–depth models through point estimates from individual dates, I propose to use the point age–depth estimates derived from the age–depth model itself, as it is based on all dating information and contains an interpretation of a likely accumulation history for a site. A robust point estimate for any depth in a core could then be provided by the weighted mean of all age-model iterations at that depth.

4. Alternative age-modelling software

Here software is presented which performs the methods detailed above simultaneously and in an automated and documented manner. The approach can be used to test the results of different age-model choices, and to systematically and rapidly produce publication-quality graphs in addition to files containing information about the settings, results, and quality of the obtained age-model. The code produces non-Bayesian, ‘classical’ age–depth models, and therefore is called clam. It can also be used to calibrate single 14C dates.

Clam has been written in the open-source statistical environment R (R Development Core Team, 2010). R can be downloaded freely at http://www.r-project.org for Windows, Mac and Linux (current version 2.10.1, c. 25 MB). The software makes use of a command-window, which may not appear very user-friendly at first sight. However, for clam the number of commands to be typed is limited. Moreover, this approach enables a highly customizable environment. R is relatively easy to learn and is being used for a growing number of applications in palaeo-research (Telford et al., 2004b; Blaauw and Christen, 2005; Heegaard et al., 2005; Blaauw et al., 2007, 2010; Haslett and Parnell, 2008). R is similar to S and clam could thus also be used in S-PLUS (Insightful Corp.). Clam comes with a manual which contains information for installing and using the code (see Section 8).

In short, clam calibrates the 14C dates (calendar scale dates such as thephras of known calendar age can be used as well), constructs an age-model based on decisions made by the user, and produces graphs and text files. Provided calibration curves are IntCal09, Marine09 (both Reimer et al., 2009) and SHCal04 (McCormac et al., 2004), while other curves such as post-bomb curves can be added. After correcting for any reservoir effect, all 14C dates of a sequence are calibrated individually through calculating their calibrated distributions for every calendar year as in Eq. (1) (default in cal BP; cal BC/AD as alternative). In case a 14C date is suspected to be outlying, it can be removed manually and is then not taken into account in the age-model. Any 14C dates which fall outside the ranges of the calibration curve will not be used, while dates which fall partly beyond its ranges will be truncated (in both cases a warning will be given). Highest posterior density probabilities are not normalised (this differs from e.g., CALIB; see Section 2). Depending on the core and chosen settings, calculations take up to c. 10–20 s on a modern PC.

Age–depth models are constructed using the calibrated distributions described above. Several common types of age-models are provided here: i) linear interpolation between the dated levels, ii) linear or higher order polynomial regression, and iii) cubic, smooth or locally weighted splines (the latter two can optionally be weighted by the inverse and squared dating errors). Sometimes the stratigraphy or the 14C dates indicate the presence of hiatuses (Blaauw and Christen, 2005); clam comes with an option to include one or more hiatuses. Extrapolation beyond the 14C dated levels is inadvisable but can be done if required.

Confidence intervals for the undated levels are calculated using the Monte Carlo approach detailed above: i) From the calibrated age distribution of every dated depth a calendar age is sampled (with the probability of a year being chosen proportional to its calibrated probability p(θ) as calculated from Eq. (1); ii) an age-model is drawn through these points, and iii) for every depth (default 1 cm steps) the resulting calendar age is stored. Per default, curves with age-reversals are rejected with a warning. In step i, an extra error term can be included akin to the mixed-effect models described in Heegaard et al. (2005); here the size of the extra error is taken to be equal to a date’s reported error. The sampling process is repeated often (default 1000 times, which suffices for most initial runs; use e.g., 10 times more iterations for final runs), resulting in as many calendar age estimates for every depth. For every depth, its calendar age point estimates are binned, ranked, normalised and summed, after which the range of those binned calendar ages which fall within e.g., 68% (1σ) or 95% (2σ) forms an estimate of the confidence interval for every individual depth. As the calculations are based on random iterations, a slightly different confidence interval will be estimated for every run.

To find the single ‘best’ age–depth model from all iterated age–depth models, clam calculates for every depth the weighted mean of all sampled calendar ages (default), or alternatively, the midpoint of the highest posterior density range of all calendar ages (default at 95% confidence intervals). In order to facilitate comparisons with commonly used although inadvisable point estimates (Table 1), clam can provide age–depth models based on i) the modes or intercepts (highest p(θ) of Eq. (1)), ii) the medians, iii) the weighted means, or iv) the midpoints of the highest posterior densities. The product of the probabilities p(θ) (see Eq. (1)) of the calendar age estimates of the dated levels provides us with a measure of the model’s goodness-of-fit. If age-reversals occur in the chosen age-model, a warning is given.

5. Case studies

Telford et al. (2004a) tested the accuracy of age–depth modelling techniques by modellng the 14C dates of a sediment sequence dated independently through varve counting. Here a slightly different approach is taken, simulating the accumulation of sediment over time and its subsequent 14C dating and age–depth modelling (Fig. 4). Sediment starts to accumulate at a rate of 20 yr/cm for the upper depth. Each depth further down has an accumulation rate differing slightly from its overlying depth, by sampling from a normal distribution with the previous accumulation rate as mean. The standard
deviation of this distribution dictates the variability in accumulation rate (here set at 7). The cumulative sum of all simulated accumulation rates then forms the accumulation history of the core. Next, a number of depths are sampled randomly from all depths (using a uniform distribution), each of which stems from a known “true” calendar year. For each of these depths, the $^{14}$C year corresponding to its calendar year is found in the IntCal09 calibration curve (Reimer et al., 2009). After adding random noise to this $^{14}$C age by sampling from a normal distribution with the $^{14}$C age as mean and 30 year as standard deviation, this value serves as a “de-calibrated” $^{14}$C age (Telford et al., 2004a). Finally clam calculates an age-depth model through the $^{14}$C dates and their depths (Fig. 4).

Generally, the age–depth models produced by clam seem to provide reasonable approximations of the true (simulated) accumulation history. Occasionally the true curve lies outside the calculated confidence intervals (Fig. 4b), but these deviations tend to occur at sections of low dating density. With more dates, the age–depth models tend to follow the true history more closely (Fig. 4c).

The effects of different age-modelling choices can be checked from a case-study; core Quilichao from a lake in Colombia (Berrio et al., 2002). This core with 9 $^{14}$C dates, and an assumed age of AD 2000 ± 5 for its surface, could be age-modelled assuming linear interpolation together with extrapolation beyond the dated levels to 800 cm (Fig. 5a). Between 485 and 445 cm depth, a large jump in $^{14}$C ages appears, suggesting a hiatus. In Fig. 5b, the age-model is linear regression, assuming a hiatus at 477 cm depth (the level where pollen spectra change abruptly; Berrio et al., 2002). In Fig. 5c, the same hiatus is assumed, and the model is based on a smooth spline. Fig. 5d, a smooth spline is drawn through all dates except the one at 445 cm which is considered an outlier.

The age-models in this example were chosen rather arbitrarily and for illustration purposes only (although the reader is reminded that at least some age–depth models in the recent literature appear to have been chosen in a similarly arbitrary way; see Table 1). Users should apply those settings which are deemed adequate for the archive in question (such as deciding between linear interpolation and polynomial or spline regression as the most likely model given the site’s deposition regime and/or stratigraphy).

6. Discussion

The software described here does not pretend to offer the latest advances in $^{14}$C modelling. Rather it attempts to provide an easy, automated, transparent, documented and adaptable environment for producing age-models from $^{14}$C sequences. Indeed, given the current suboptimal approaches and lack of information in most published age–depth models (Table 1), it is hoped that clam could aid in standardising and enhancing future ‘classical’ age–depth models.

Other software exists for producing age-models of $^{14}$C dated sequences. In psimpoll (Bennett, 2008) one can choose from a large number of age-models, but $^{14}$C dates are left uncalibrated or need to be calibrated outside the program (e.g., in BCal; Buck et al., 1999), and hiatuses cannot be included. Tilia (Grimm, 1990) is popular for age–depth model construction, but cannot handle hiatuses or asymmetric dates, and does not take into account the errors of dates. Heegaard et al. (2005) provide R code for $^{14}$C age-modelling based on mixed-effect regression, but there calibrated $^{14}$C dates are assumed to have a normal distribution on the calendar scale, hiatuses are not taken into account, and only one type of age-model can be chosen. Blaauw and Christen (2005) published Bayesian software Bpeat for ‘wiggle-matching’ $^{14}$C dates based on the age-model of piece-wise linear accumulation; other age-models are not included in their program. OxCal (Bronk Ramsey, 2008) provides a number of age–depth models based on Bayesian statistics, and recently Bayesian software based on a monotonous accumulation model has been published (Haslett and Parnell, 2008).

The Bayesian age-modelling routines mentioned in the previous paragraph (Blaauw and Christen, 2005; Bronk Ramsey, 2008; Haslett and Parnell, 2008) use advanced, robust and flexible numerical methods, and should be the preferred approach for future age–depth models (Blockley et al., 2007). However, we have seen that many studies continue to apply ‘classical’ age–depth modelling routines, and existing Bayesian age–depth modelling methods might not add much extra value to low-resolution dated sites. Therefore, the intended use of clam is to rapidly, transparently and systematically produce age-models, while exploring the impact of different modelling choices (e.g., type of age-model, presence or
absence of a hiatus, reservoir effect, outliers, or anchor points). As a next step in the age-modelling process, more sophisticated approaches relevant for the core in question should be considered (Blockley et al., 2007).

It is vital to note the dangers of reducing calibrated $^{14}$C dates to single-year point estimates and subsequent drawing of a single age–depth curve through these points. Point age estimates of calibrated $^{14}$C dates and undated levels should not be regarded as the truth (e.g., see Telford et al., 2004b; Michczyński, 2007; Blaauw et al., 2007; Scott, 2007). Rather much attention should be paid to the estimated uncertainties for both the calibrated dates and the entire sequence.

The R code of clam can be understood relatively easily. Indeed, users are invited to adapt the code to their preferences, such as the figure settings. The open nature of the code enables the interested user to open the ‘black box’ of age-modelling, following in detail how $^{14}$C dates can be calibrated and age-models derived. With this in mind, clam is also of use for educational purposes.

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Appendix. Supplementary information

Supplementary information associated with this article can be found, in the online version, at doi:10.1016/j.quageo.2010.01.002 and http://chrono.qub.ac.uk/blaauw/.

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