

# Estimating radiocarbon calibration curves

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**Abstract.** In addition to being crucial to the establishment of archaeological chronologies, radiocarbon dating is vital to the establishment of time lines for many Holocene and late Pleistocene palaeoclimatic studies and palaeoenvironmental reconstructions. The calibration curves necessary to map radiocarbon to calendar ages were originally estimated using only measurements on known age tree-rings. More recently, however, the types of records available for calibration have diversified and a large group of scientists (known as the IntCal Working Group—IWG) with a wide range of backgrounds has come together to create internationally-agreed estimates of the calibration curves. In 2002, Caitlin Buck was recruited to the IWG and asked to offer advice on statistical methods for curve construction. In collaboration with Paul Blackwell, she devised a tailor-made Bayesian curve estimation method which was adopted by the IWG for making all of the 2004 internationally-agreed radiocarbon calibration curve estimates. This paper reports on that work and on the on-going work that will eventually provide models, methods and software for rolling updates to the curve estimates.

## 1 Introduction

### 1.1 Radiocarbon dating

Carbon is one of the most abundant elements and, due to its capacity to bond with other elements, it is a vital part of all living organisms. As a result, in the late 1940s, when Willard Libby and colleagues discovered a method for estimating the age of carbon-containing materials there was great excitement in a number of disciplines including archaeology, geology and palaeontology.

Libby's method relies on the fact that one of the isotopes of carbon— $^{14}\text{C}$ —is radioactive. While they are alive, all plants and animals exchange carbon (including  $^{14}\text{C}$ ) with the atmosphere. This means that, during life, living organisms have levels of  $^{14}\text{C}$  that are in approximate equilibrium with the atmosphere. Upon death, however, plants and animals cease metabolising and so no new carbon is taken up. At this point, the amount of  $^{14}\text{C}$  in any surviving tissue begins to decrease exponentially, via radioactive decay.

If we assume, as Libby and colleagues did, that the ratio of  $^{14}\text{C}$  to other carbon isotopes has been constant over time then all we need to date a sample of (long) dead carbon are: an estimate of the proportion of  $^{14}\text{C}$  in modern carbon, an estimate of the half-life of  $^{14}\text{C}$  and a method to estimate the current proportion of  $^{14}\text{C}$  in the sample itself. Libby and colleagues provided all of these and so radiocarbon dating appeared both simple and reliable. It also appeared particularly useful to archaeologists since Libby's estimate of the half-life was  $5568 \pm 30$  years; i.e. about right to help date most

of the human past. The current estimate of the half-life is  $5730 \pm 40$  years, but to avoid confusion (given the need for calibration explained below) all radiocarbon laboratories still use the Libby half-life to calculate radiocarbon ages.

## 1.2 The Need for Calibration

As discussed in some detail in Aitken (1990) and Bowman (1990), quite quickly after radiocarbon dating was discovered, it became clear that Libby's assumption of constant  $^{14}\text{C}$  levels in the atmosphere does not hold. The level is affected by very many complex factors that have proven impossible to model mechanistically. These include natural factors such as: solar cycles, solar storms, geomagnetic variations in the earth and unpredictable up-welling of old carbon from substantial reservoirs such as oceans. The level has also been impacted by human activity; for example, it increased substantially due to atomic bomb testing in the 1950s and has dropped again more recently due to release of old carbon in fossil fuels.

As a consequence, radiocarbon dating is only viable if we can obtain an estimate of the varying level of  $^{14}\text{C}$  back through time and can thus plot the function that links radiocarbon ages to calendar ages. Put loosely, we need a calibration curve. Since the factors affecting variations in  $^{14}\text{C}$  level are too complex to model mechanistically the only way to get such a curve is to estimate it from data.

## 1.3 The Calibration Curve

Given a radiocarbon determination  $X_0$  for a sample, we wish to assess the true age  $\theta_0$  of the sample by taking into account the information from other samples of known (or approximately known) age, our 'calibration data', which are paired radiocarbon determinations and calendar ages  $\mathcal{X} = (X_1, \dots, X_N)$  and  $\mathcal{T} = (T_1, \dots, T_N)$ . That is, we are interested in

$$p(\theta_0 | \mathcal{X}, \mathcal{T}, X_0).$$

An object of age  $\theta$  has 'true' radiocarbon determination  $\mu(\theta)$  say, so that  $E(X_0 | \theta_0) = \mu(\theta_0)$ , and furthermore  $X_0$  depends on  $\mathcal{X}$  and  $\mathcal{T}$  only through  $\mu(\cdot)$ . Thus, although it was not articulated in this way originally, at the core of the radiocarbon dating method is a process that can be summarised by the function  $\mu(\cdot)$ , the so-called 'calibration curve'. We can write

$$p(\theta_0 | \mathcal{X}, \mathcal{T}, X_0) = \int p(\theta_0 | \mu, X_0) p(\mu | \mathcal{X}, \mathcal{T}, X_0) d\mu. \quad (1)$$

This paper primarily concerns inference about  $\mu(\cdot)$ . Calculation of  $p(\theta_0 | \mu, X_0)$  and the integral (1), and hence the actual calibrating of an individual date, are addressed only briefly in Sections 2, 6.6 and 7.

## 2 Historical background

The work reported in this paper builds on research by a large number of people (some very famous and many unrecognised) in several disciplines who have contributed to making radiocarbon dating ubiquitous. The first of these was Willard Libby (1908 to 1980) whose role in developing radiocarbon dating (Anderson et al., 1947; Libby et al., 1949; Arnold and Libby, 1949) led to him being awarded the Nobel Prize for chemistry in 1960. The discovery of the method was followed by several years of work by a number of other people who noted that the initial assumption of constant atmospheric radiocarbon ( $^{14}\text{C}$ ) levels seemed to be erroneous and, hence, that there is a need for calibration of radiocarbon ages onto the calendar scale (e.g. de Vries, 1958 and Willis et al., 1960).

Pivotal early work on estimating  $p(\mu(\cdot)|\mathcal{X}, \mathcal{T})$  was undertaken by the influential physical chemist Hans Suess (1909 to 1993) who radiocarbon dated samples of trees that had already been calendar dated using tree-ring dating (dendrochronology). Plotting the resulting paired points, he hand-drew a “calibration” curve using a method that he called “cosmic schwung” (Suess, 1967, 1970). Since then there have been continuous attempts to provide more reliable estimates of the relationship between radiocarbon and calendar age back over the entire period for which radiocarbon dating is viable (i.e. to about 55,000 or 60,000 years ago).

What has been clear since the very early work, is that the relationship is non-monotonic and so a single radiocarbon age often maps to multiple calendar ages. The non-monotonicity of this curve is one of the reasons that statisticians have, for so long, regarded radiocarbon dating as an interesting source of case studies. Indeed a statistician, Malcolm Clark (then in the Department of Probability and Statistics at the University of Sheffield, now at Monash), was highly influential in some of the early work on radiocarbon calibration curve estimation. He used the curve estimation problem as a case study in non-parametric curve fitting (Renfrew and Clark, 1973, 1974) and, on at least one occasion (Clark, 1975), gave considerable, tailored advice to radiocarbon scientists about error estimation. More recently, an over-growing collaborative team has sought to provide internationally-agreed estimates of calibration curves. Until recently, this group did not include a statistician and they used rather *ad hoc* procedures that involved taking weighted averages of calibration data in predefined windows and then using piece-wise linear or spline fits to create the curves (Pearson and Stuiver, 1986; Stuiver and Pearson, 1986a; Pearson and Stuiver, 1993; Stuiver and Pearson, 1993; Stuiver et al., 1998).

Once radiocarbon calibration curve estimates became routinely available, archaeologists and other researchers began to seek ways to obtain  $p(\theta_0|\mu(\cdot), X_0)$ . Since the radiocarbon dating laboratories provide only estimates of  $X_0$  (of the form  $x_0 \pm \sigma_0$ ) and we do not know  $\mu(\cdot)$  precisely, this is clearly a statistical problem. The pioneering work in developing calibration algorithms and software was undertaken by radiocarbon scientists (e.g. Stuiver and Reimer, 1986), but quite quickly statisticians started to see this as an interesting area of work. By 1989, when sufficient work had been done in this area to merit a review article (Aitchison et al., 1989), several statisticians were involved; in particular Tom Aitchison and Marian Scott (University of Glasgow) and Morven Leese

(then at the British Museum Research Laboratory, now at Kings College, London).

At that time there were, broadly speaking, two methods being used for calibration. The “intercept method” was popular in the early days because it could be implemented by anyone with access to a plot of the calibration curve at an appropriate scale. It simply involved drawing lines from the radiocarbon axis to intercept with the curve and then reading off the related calendar age(s) (Stuiver and Pearson, 1986b). Since lines could be drawn at any point, both point estimates and estimates of confidence intervals were provided using this method. The alternative method, known as the “probability distribution method” was only practical for those with access to computing resources. Stuiver and Reimer (1989) discuss a range of options for estimating full probability distributions of calendar ages given the non-monotonic calibration curve.

At about this time, Bayesian statisticians were beginning to join the debate. Indeed even before the Aitchison et al. (1989) review was published, the pioneering paper which laid the groundwork for future research in Bayesian radiocarbon calibration had already been published. John Naylor (Nottingham Trent University) and Adrian Smith (then at University of Nottingham, now Principal at Queen Mary, University of London and elected Fellow of the Royal Society in 2001) were introduced to the interesting statistical challenges posed by radiocarbon calibration by Clive Orton (University College London, Institute of Archaeology), a statistician with considerable archaeological experience who could see the merits of formally utilising prior information in radiocarbon calibration. The paper that arose from this (Naylor and Smith, 1988) is very detailed, offering a fully Bayesian modelling framework for radiocarbon calibration, not just for single radiocarbon determinations but for groups of related phases and sequences of determinations from a single archaeological site.

Within the radiocarbon literature debates about the right way to calibrate continued, but convergence towards the adoption of a generally Bayesian approach was happening relatively quickly. It took another statistician, Herold Dehling (then at University of Gröningen, now at Ruhr-Universität Bochum) in collaboration with an influential radiocarbon scientist, Hans van der Plicht (University of Gröningen), to explain clearly to the radiocarbon community what formal options they had for calibration and why the Bayesian approach (formulated in the way advocated by Naylor and Smith, 1988) was superior to other approaches suggested in the past (Dehling and van der Plicht, 1993).

Meanwhile, major developments were occurring in the Bayesian statistics research community. Adrian Smith (then still at University of Nottingham), in collaboration with Alan Gelfand (then University of Connecticut, now Duke University), following earlier work in this area by others including Geman and Geman (1984), drew attention to a number of simulation tools (stochastic substitution, Gibbs sampling and sampling-importance-resampling) for calculating numerical estimates of marginal posterior probability distributions (Gelfand and Smith, 1990). With this work the so called MCMC (Markov chain Monte Carlo) “revolution” in Bayesian inference began.

By chance, at this time both of the present authors were also in Nottingham. One of us (CEB) was working as a research assistant on a joint research project, between the Departments of Archaeology and Mathematics, that was coming to an end and so was

seeking further employment. Adrian Smith was looking for eager programmers to work on case studies in the use of MCMC in Bayesian inference and so began the on-going work to provide archaeologists and other researchers with the tools that they needed to do fully Bayesian radiocarbon calibration (Buck et al., 1991, 1992, 1994a,c,b; Buck and Litton, 1995; Zeidler et al., 1998; Blackwell and Buck, 2003).

Thus, radiocarbon dating was a research problem in the right place at the right time and it was one of the very first complex statistical problems to benefit from the application of Bayesian inference via MCMC. For this reason it is one of the major case studies in the pivotal book *MCMC in Practice* (Gilks et al., 1996) and two Bayesian radiocarbon calibration packages (BCal and OxCal) are now routinely used by archaeologists in their research (Buck et al., 1999; Bronk Ramsey, 1995, 2001). Indeed, the use of Bayesian statistics in radiocarbon calibration is now so well established that it was recently used as a case study by a philosopher of science. Daniel Steel (Michigan State University), used some of the work cited above, in an on-going debate in the philosophy of science about whether or not scientists reason partially, and therefore operate, as Bayesians (Steel, 2001).

So why is it, more than ten years after the first routine use of Bayesian methods in radiocarbon calibration, that this topic is still worthy of being treated as a major case study in Bayesian statistics? The answer is simple. Until relatively recently Bayesian statisticians only paid attention to developing methods for estimating  $p(\theta_0|\mu(\cdot), X_0)$ ; assuming that the calibration function,  $\mu(\cdot)$ , is well understood. In practice, however, this is far from the case and since 2002, when CEB joined the IntCal Working Group, which provided the 2004 internationally-agreed estimates of the radiocarbon calibrations curves (Reimer et al., 2004; Hughen et al., 2004; McCormac et al., 2004) substantial efforts have been made to bring modern Bayesian methods to bear upon inference for curve estimation as well. It is this work that forms the focus of what follows.

### 3 The calibration data

Before we can talk in detail about Bayesian methods for calibration curve estimation, we need to be clear what form the available calibration data take. As mentioned above, early curve estimates relied on radiocarbon dating lots of samples of trees that had previously been calendar dated via dendrochronology. Since tree-ring dating is assumed to give calendar ages that are reliable to the nearest year (and a calibration curve to the nearest year was considered more than adequate), researchers assumed that the only uncertainty associated with such data were the laboratory's estimates of their in-house errors on the radiocarbon measurements. Treating calendar age as the explanatory variable and radiocarbon age as the dependent variable meant that lots of standard curve fitting methods could be used. Unfortunately, however, this summary of the nature of the data belies an important complication that is present in most such data.

In practice, although tree-ring dating does provide a precise calendar date for each ring in each tree, there is not enough  $^{14}\text{C}$  in a single ring to allow a reliable estimate of the radiocarbon age to be established by conventional (as opposed to atomic mass

spectroscopy) radiocarbon dating laboratories. Consequently, for most calibration curve projects blocks of timber containing 10 or 20 rings are sent for radiocarbon dating. It is this blocked nature of the data which led to the use of an *ad hoc* window-based method to calculate weighted averages for the 1993 and 1998 internationally-agreed radiocarbon calibration curves. As we will see, in 2004 we took account of this structure by formal modelling.

Recently a desire to provide calibration data back beyond the end of what is practical for tree-ring dating (currently around 12,000 years before present) has led to a search for other materials that can provide both calendar and radiocarbon date estimates. As a result, the 2004 IntCal database (available at <http://www.radiocarbon.org/IntCal04.htm>) contains data derived from trees, but also from corals and from sequentially deposited lake/ocean sediments. Calcite from corals can be radiocarbon dated and calendar age estimates are usually obtained by uranium-series dating; also known as uranium/thorium (or U/Th) dating—another dating method that relies on radioactive decay, but that does not require calibration. For sedimentary sequences, calendar date estimates are either obtained by counting annual laminae or varves (just like tree-rings) or by an age/depth model where such laminae do not exist; trapped carbonaceous material such as foraminifera (small marine creatures that build a delicate house, called ‘test’, from calcite), are the selected from some layers and sent for radiocarbon dating. One of the important data sets for IntCal04 (Hughen et al., 2004) comprises laminated sediments, but does not have laminae all the way up to the present day. As a result, we know how many years are in the sample, but not when each layer was deposited. Such sequences—known as “floating” sequences—need to be tied into another record for which the calendar ages are known. This process of tying records together is known as “sequence matching” or “wiggle matching” and brings with it extra uncertainty in addition to that arising from the counting of annual laminae.

Clearly, each of these methods for obtaining calendar ages results in quite different error structures, some of which are highly correlated, that need to be carefully modelled in any formal curve estimation process.

## 4 The prior for $\mu(\cdot)$

Our prior beliefs about  $\mu(\cdot)$  are crucial to the whole process of calibration. The use of calibration data makes sense only because we believe that  $\mu(\theta)$  does not change too quickly with  $\theta$ . We expect that  $\mu(\cdot)$  should change fairly slowly over time, representing gradual changes in radiocarbon levels in the atmosphere. In fact, what we refer to here as “radiocarbon determinations” are not ‘raw’ ratios of carbon isotopes, but have been transformed onto an approximate timescale, by convention, in a way that would produce true ages if the original assumption of constant atmospheric radiocarbon were correct. (Some literature still refers to these as “radiocarbon ages”.) We therefore might expect  $\mu(\cdot)$  to change by approximately one (radiocarbon) year per (calendar) year.

We can represent these beliefs using a Wiener process, with drift  $\beta$  and variance  $r^2$

(per year), relating radiocarbon determinations at ages  $\theta$  and  $\theta'$  by

$$\mu(\theta')|\mu(\theta) \sim N((\theta' - \theta)\beta, (\theta' - \theta)r^2), \theta' > \theta.$$

In practice, since we wish to avoid the level of detailed modelling necessary to allow for intra-annual effects, we can use the natural annual time scale and think of  $\mu(\cdot)$  at integer ages only, with a prior given by a random walk with increments

$$Z_i \sim N(\beta, r^2).$$

## 5 Pointwise Estimation of the Calibration Curve

### 5.1 Introduction

In this part of the paper, we describe the method actually used to estimate  $\mu(\cdot)$  for the 2004 internationally-agreed Northern hemisphere terrestrial calibration curve (Buck and Blackwell, 2004; Reimer et al., 2004). Extensions to this method (which are not discussed further here, but are documented in Buck and Blackwell, 2004) were used to provide the internationally-agreed marine calibration curve Hughen et al. (2004) and the internationally-agreed Southern Hemisphere terrestrial calibration curve McCormac et al. (2004). The development of the models and methods, and the actual calculations required to provide the 2004 estimates, were undertaken by the present authors, closely guided by the IntCal Working Group of which CEB was a member.

At a meeting of the IntCal Working Group (IWG) at Queen's University Belfast (in 2002) criteria were agreed for the inclusion of calibration data which led to acceptance of datasets with the properties described in Section 3 (and documented in greater detail in Reimer et al., 2002). At a second meeting at the Woods Hole Oceanographic Institute (in 2003) the IWG also laid down some requirements for the statistical approach. In particular, having been encouraged by CEB and others at the Belfast meeting to quantify uncertainty on the calendar ages of the calibration data, the group were very keen that these should—for the first time—be taken into account. The IWG, which is composed mostly of laboratory physicists, also felt quite strongly that the statistical procedures should use an explicit repeatable numerical method (as opposed to a simulation-based approach). Finally, since it was not in the remit of the IWG to provide new software for radiocarbon calibration, it was also agreed that the final curves should be reported in the same form as previous ones; i.e. as posterior means and standard deviations for points  $\mu(\theta)$  on the curve at selected regularly spaced values of  $\theta$ .

The requirement of a numerical approach imposed some limits on what could be achieved on a timescale that was judged worthwhile, given the pressure from the radiocarbon dating user community for a curve that made use of the latest data. In particular, it was agreed, early on, that in representing prior beliefs of the form described in Section 4, it was not feasible to treat  $r$  as unknown, with uncertainty represented through a hyper-prior; instead,  $r$  needed to be fixed. Details of how a value was chosen are given in Section 5.5.

On the other hand, the decision to limit the output to means and variances meant that our calculations could treat separately each required point on the curve. This had the practical advantage that we could limit the observations to be considered in any one calculation to a fraction of the whole data set. This involves an element of approximation, but for each point on the curve we chose a suitable window so that this effect was negligible; see Section 5.5 for details. Of course, calculating points on the calibration curve separately has the disadvantage that it does not give the posterior covariances between the estimated points. However, given the way in which the curves are routinely used for calibration, it was judged that these covariances were unlikely to be used even if reported. This issue is revisited in Section 6.6.

For each calendar date  $\theta^*$  at which we wish to estimate the curve, we choose a subset of the observations,  $X_1, \dots, X_N$ , from dates in a suitable window around  $\theta^*$ . As shown below, we can then approximate the joint distribution of  $X_1, \dots, X_N$  given  $\mu(\theta^*)$  by a multivariate normal distribution, and invert this numerically to get a posterior mean and standard deviation for  $\mu(\theta^*)$ . This gives the required information at each point on the curve.

Specific models for  $X_j|\mu(\theta^*)$  corresponding to the various kinds of calibration data are discussed in the following Sections 5.2 to 5.4. Some practical details of the implementation are discussed in Section 5.5.

## 5.2 Modelling the calibration data - the simplest case

A standard assumption is that a radiocarbon determination,  $X_j$ , is an observation of the ‘true’ radiocarbon age of object  $j$  with an error,  $\epsilon_j$ , made up of the laboratory’s estimate of its internal error with variance  $s_j^2$  say and what is known as a laboratory error multiplier,  $k_l$  say, which allows for inter-laboratory variability and for IntCal04 was explained in Reimer et al. (2004), pp. 1034–1035. In the simplest case, the calibration data come from samples of genuinely known date, so that  $T_j = \theta_j, j = 1, \dots, N$ , and are independent, with

$$\begin{aligned} X_j &= \mu(\theta_j) + \epsilon_j, \quad j = 1, \dots, N \\ \epsilon_j &\sim N(0, \sigma_j^2), \quad j = 1, \dots, N \end{aligned}$$

where  $\sigma_j^2 = k_l^2 s_j^2$ . If we wish to evaluate the curve at  $\theta^*$  say we then have

$$X_j \sim N(\mu(\theta^*) + (\theta_j - \theta^*)\beta, |\theta_j - \theta^*|r^2 + \sigma_j^2). \quad (2)$$

Note that the  $X_j$ s are *not* independent conditional on  $\theta^*$  since the uncertainty in  $\mu(\cdot)$  is common to multiple observations. The covariance between two observations  $X_i$  and  $X_j$ , conditional on  $\theta^*$ , is

$$\text{Cov}(X_i, X_j) = r^2(\min\{\theta_i, \theta_j\} - \theta^*) \quad (3)$$

if  $\theta_i, \theta_j > \theta^*$ , with a similar expression if  $\theta_i, \theta_j < \theta^*$  and zero covariance otherwise.



In practice, for each date  $\theta^*$  at which we wish to estimate the curve, we select those observations  $X_1, \dots, X_N$  associated with calendar dates in a suitable window around  $\theta^*$ . Then  $X_1, \dots, X_N$  given  $\mu(\theta^*)$  have a multivariate normal distribution with mean equal to  $\mu(\theta^*)\mathbf{1}$  and covariance given above. With a uniform (or indeed any Gaussian) prior for  $\mu(\theta^*)$ , it is then straightforward to obtain a posterior estimate for  $\mu(\theta^*)$  and an associated standard deviation (inverting the covariance matrix numerically).

In this simplest case, the approach described here is related to the approaches of Christen and Nicholls (2000), Gómez Portugal Aguilar et al. (2002) and Buck et al. (2006). However, if we are to allow for the real complexity of uncertainty and dependence in the calibration data, as described in Section 3, then we need to represent a more general structure in the data.

### 5.3 Averaging over blocks

A single determination  $X_j$  may arise not from material from a single precise date, but from an average over successive years e.g. blocks of consecutive tree-rings. Extending the calculations to this case is straightforward in principle. In practice, we carry out the calculation by exploiting the natural annual time scale, since each  $X_j$  is a linear combination of  $\mu(\theta)$ s, and any change in  $\mu(\cdot)$  is a sum of increments  $Z_\theta$  indexed by (integer) date  $\theta$ . As before, we use the  $X_j$ s associated with calendar dates in some ‘window’  $(\theta_{\min}, \theta_{\max})$  around  $\theta^*$ . We write

$$\mathbf{X} = \begin{pmatrix} X_1 \\ \vdots \\ X_N \end{pmatrix}, \quad \boldsymbol{\varepsilon} = \begin{pmatrix} \epsilon_1 \\ \vdots \\ \epsilon_N \end{pmatrix}, \quad \mathbf{M} = \begin{pmatrix} \mu(\theta_{\min}) \\ \vdots \\ \mu(\theta^*) \\ \vdots \\ \mu(\theta_{\max}) \end{pmatrix}, \quad \mathbf{Z} = \begin{pmatrix} -Z_{\theta_{\min}+1} \\ \vdots \\ -Z_{\theta^*} \\ Z_{\theta^*+1} \\ \vdots \\ Z_{\theta_{\max}} \end{pmatrix}.$$

Then

$$\mathbb{E}[\mathbf{X}] = \mathbf{A}\mathbf{M},$$

where the matrix  $\mathbf{A}$  defines the contributions of different years to each sample. In practice, we typically have equal weights over  $n_j$  successive years for the  $j$ th sample, so  $a_{j,\theta} = n_j^{-1}$  if  $\theta_j \leq \theta \leq \theta_j + n_j - 1$  and  $a_{j,\theta} = 0$  otherwise. We can further write

$$\mathbf{M} = \mathbf{B}\mathbf{Z}$$

where the matrix  $\mathbf{B}$  is of the form

$$\begin{pmatrix} 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 1 & 1 & 1 \end{pmatrix},$$

extended to cover the range  $(\theta_{\min}, \theta_{\max})$ , and so

$$\mathbf{X} = \mathbf{ABZ} + \boldsymbol{\varepsilon}$$

where the matrix  $A$  is defined by  $a_{j,\theta} = n_j^{-1}$  if  $\theta_j \leq \theta \leq \theta_j + n_j - 1$  and  $a_{j,\theta} = 0$  otherwise.

The approach described so far enables us to estimate individual points on the calibration curve at dates where error on the calendar scale is negligible—essentially those using tree-ring data only. In particular, this approach suffices for the most recent parts of IntCal04 (Reimer et al., 2004), back to 12,400 years before present.

## 5.4 Uncertainty in calendar dates

### Means and variances

Often in practice (for example when U/Th dating is used) we do not observe  $\theta_j$  directly, but instead observe

$$T_j \sim N(\theta_j, \tau_j^2).$$

Given a flat (improper) prior distribution for  $\theta_j$ , this implies

$$\theta_j | T_j \sim N(T_j, \tau_j^2).$$

Then  $X_j | T_j$  has mean

$$\mu(\theta^*) + (T_j - \theta^*)\beta$$

and variance

$$r^2 \mathbb{E}[(\theta_j - \theta^* | T_j) + \sigma_j^2],$$

which can be calculated analytically when  $\theta_j \sim N(T_j, \tau_j^2)$ .

### Covariances: independent calendar ages

The corresponding covariance between observations  $X_i$  and  $X_j$  is straightforward if we make the assumptions that  $T_i$  and  $T_j$  are independent and that  $\theta_i$  and  $\theta_j$  are independent, *a priori* and hence conditional on  $T_i$  and  $T_j$ . This is natural if for example the observations relate to completely separate data sources, or are directly dated using U/Th dating.

In such cases,  $\text{Cov}(X_i, X_j)$  involves

$$\mathbb{E}[c(\theta_i - \theta^*, \theta_j - \theta^*) | T_i, T_j]$$

where

$$c(\phi, \psi) = \begin{cases} \min\{|\phi|, |\psi|\} & \text{if } \phi, \psi \text{ have the same sign,} \\ 0 & \text{otherwise.} \end{cases}$$

This expectation cannot be evaluated analytically, but can be obtained readily by numerical integration.

### Covariances: dependent calendar ages

The corresponding covariance between observations  $X_i$  and  $X_j$  is more complicated if the uncertainties in  $\theta_i$  and  $\theta_j$  are linked, for example if they have some layer-counting or sequence matching error in common.

For example, if  $X_i$  and  $X_j$  are in the same ‘floating’ sequence of observations, assigned absolute dates by wiggle-matching, then any wiggle matching error,  $\omega$ , will be common to the two, and so we might have

$$\begin{aligned} T_i &= \theta_i + \omega, \\ T_j &= \theta_j + \omega, \\ \omega &\sim N(0, \tau^2) \end{aligned}$$

if there is no other calendar age error. If, on the other hand,  $T_i$  and  $T_j$  are determined by layer counting within the same varved sequence, and  $T_i < T_j$ , then any error accrued up to layer  $T_i$  will also affect  $T_j$ , and we might have

$$\begin{aligned} T_i &= \theta_i + \omega_i, \\ T_j &= \theta_j + \omega_i + \omega_j \end{aligned}$$

where both  $\omega_i$  and  $\omega_j$  have Poisson distributions that, like the radiocarbon counting errors, can be approximated by normal distributions for present purposes.

In general, we assume that

$$\theta_i, \theta_j | T_i, T_j$$

is bivariate normal, as above, and then numerical integration can still be used to evaluate  $\text{Cov}(X_i, X_j)$ .

A final example of dependence structures that we need to represent arises when, as well as having calendar date estimates, we know *a priori* that certain observations are ordered in time. For example, the sedimentary sequences described in Section 3 have annual layers (‘laminae’) whose ordering is known and should be incorporated in the analysis. Representing a strict ordering is not easy within the current framework, although it is straightforward in the more flexible approach described in Section 6). The estimated calendar dates of these layers respect the ordering, of course; for the moment, we simply add a strong positive correlation between the errors on the dates, as an approximate representation of the ordering.

The cases described in this section complete the range of error structures needed to permit a coherent, if in places approximate, representation of all the data available for the estimation of the older part of IntCal04 Reimer et al. (2004) from 12,400 to 26,000 years before present.

## 5.5 Implementation for IntCal04

### Specifying the random walk

The implementation outlined in Section 5.1 depends crucially on specifying the prior for  $\mu$ , as described in Section 4, in terms of fixed numerical values for the mean  $\beta$  and variance (per year)  $r^2$ .

As indicated in Section 4, it seems natural to take  $\beta = 1$ , since that corresponds to the calibration curve changing by approximately 1 (radiocarbon) year per (calendar) year. In practice, however, the results are very robust to changes in  $\beta$ ; even taking  $\beta = 0$ , which simplifies the calculations slightly, makes a negligible difference to the curve that we obtain.

In contrast, the value of the variance  $r^2$  can make a real difference to the curve, so care is needed in setting this parameter. Christen and Nicholls (2000) estimated a value of  $r = 7.9$  using single year data from Stuiver et al. (1998). In a similar way, we used high-resolution subsets of the IntCal04 data to estimate  $r$ . In the light of both sets of experiments, for the actual production of the curve in Reimer et al. (2004) we took  $r = 8$ .

### Choosing the window

Before final production of the IntCal04 curve, we experimented at length with the choice of window for data selection. In most parts of the curve, it was sufficient to use the 100 observations  $X_j$  with values  $T_j$ , or  $\theta_j$  if known, closest to  $\theta^*$ . For a small part of the curve where there were many observations with large errors, it was necessary to use the nearest 200 points to estimate  $\mu(\theta^*)$  accurately.

### Choosing output values

Since the curve was to be reported as a discrete set of points, we needed to choose an actual set of values of  $\theta^*$  to use. For the most recent part of the curve, we chose to report values at 5 year intervals, which seemed to be fine enough to represent essentially all of the information in the data and which was compatible with the 10 year intervals with which users are familiar from IntCal98. Older parts of the curve are reported more sparsely, in view of the decreased density of the data and the increased calendar-age error.

It is worth emphasising that using the approach described, the curve can be evaluated at any point  $\theta^*$ , by contrast with earlier approaches where the spacing of points was built in to the method used.

### Numerical integration

The calculation of covariances between observations, given calendar age error as in Section 5.4, requires evaluating the expectation of

$$c(\phi, \psi) = \begin{cases} \min\{|\phi|, |\psi|\} & \text{if } \phi, \psi \text{ have the same sign,} \\ 0 & \text{otherwise} \end{cases}$$

when  $\phi, \psi$  have a bivariate normal distribution, by numerical integration. For IntCal, a rather crude method was used; evaluating  $c(\cdot, \cdot)$  on a regular  $25 \times 25$  grid, suitably centred, gave an adequate approximation.

## 6 A Markov chain Monte Carlo approach

The requirements of the IntCal Working Group, as described in Section 5.1, precluded simulation-based calculation of the curve at that time. However, during the process of modelling and calculation it became clear that there were a number of potential advantages of such an approach. In particular, a Markov chain Monte Carlo (MCMC) approach can incorporate uncertainty about the random walk variance  $r^2$  and allows us to obtain posterior covariances between points on the curve, as well as estimates and standard deviations for any other aspect of the curve. We now describe how a curve can be constructed using MCMC, and briefly explore some consequences.

### 6.1 Preliminaries

We denote the true ages of the calibration samples by  $\Theta = (\theta_1, \dots, \theta_N)$ , and write  $\mathcal{M} = (\mu_1, \dots, \mu_N) = (\mu(\theta_1), \dots, \mu(\theta_N))$ . We write  $\mathcal{M}_{(j)}$  for the vector with elements  $\mu_i, i \neq j$ , and similarly for the  $\theta$ s.

Our approach will be to exploit the fact that the calibration data give direct information on the curve only at the particular, perhaps unknown, dates to which they relate; this follows from the Markov nature of our prior for  $\mu(\cdot)$ . Thus

$$p(\mu|\mathcal{X}, \mathcal{T}) = \int p(\mu|\mathcal{M}, \Theta)p(\mathcal{M}, \Theta|\mathcal{X}, \mathcal{T})d\mathcal{M}d\Theta. \quad (4)$$

A crucial standard result for both terms in the integral in equation 4, which follows from modelling the curve as a Wiener process, is that the conditional distribution of  $\mu(\theta^*)$  say is

$$\mu(\theta^*)|\mathcal{M}, \Theta, r \sim N(\mu^B + (\mu^A - \mu^B)\phi, r^2(\theta^A - \theta^B)\phi(1 - \phi)) \quad (5)$$

where

$$\begin{aligned}\theta^A &= \min\{\theta \in \Theta : \theta \geq \theta^*\} \\ \theta^B &= \max\{\theta \in \Theta : \theta \leq \theta^*\} \\ \mu^A &= \mu(\theta^A) \\ \mu^B &= \mu(\theta^B) \\ \phi &= \frac{\theta^* - \theta^B}{\theta^A - \theta^B}.\end{aligned}$$

To make inference about  $\mathcal{M}$  based on observations  $\mathcal{X} = \{X_1, \dots, X_N\}$ , we have

$$\mu_j | \mathcal{M}_{(j)}, \Theta, \mathcal{X}, r \sim N\left(\frac{x_j/\sigma_j^2 + \mu_{RW}/\sigma_{RW}^2}{1/\sigma_j^2 + 1/\sigma_{RW}^2}, \frac{1}{1/\sigma_j^2 + 1/\sigma_{RW}^2}\right) \quad (6)$$

where  $\mu_{RW}$  and  $\sigma_{RW}^2$  are the mean and variance on the RHS of equation 5 when used to calculate  $\mu_j | \mathcal{M}_{(j)}, \Theta, r$ .

## 6.2 Known-age calibration samples

The results in Section 6.1 are enough to allow inference about the curve in the absence of calendar age errors, the equivalent of Section 5.2. Equation 6 can be used for a Gibbs sampling approach to imputing  $\mathcal{M}$ , since it gives the full conditional distributions  $\mu_j | \mathcal{M}_{(j)}, \Theta, r$ .

We do not cover here the case of ‘blocking’ of observations, as in Section 5.3. This situation is straightforward but rather intricate within the MCMC approach, because of the need to cover various cases of overlapping blocks in generalising equation 5.

It is straightforward also to include a Gibbs sampling step for  $r | \mathcal{M}, \Theta$ , allowing the more general form of prior in which  $r$  is treated as unknown.

## 6.3 Independent calendar age errors

If our observations have uncertainty on the time axis, we use a Metropolis-within-Gibbs algorithm that updates each  $(\theta_j, \mu_j)$  together. First, write

$$\begin{aligned}& p(\theta_j, \mu_j | \mathcal{X}, \mathcal{T}, \mathcal{M}_{(j)}, \Theta_{(j)}, r) \\ &= p(\mu_j | \theta_j, x_j, \mathcal{M}_{(j)}, \Theta_{(j)}, r) p(\theta_j | x_j, t_j, \mathcal{M}_{(j)}, \Theta_{(j)}, r) \\ &\propto p(\mu_j | \theta_j, x_j, \mathcal{M}_{(j)}, \Theta_{(j)}, r) p(x_j | \theta_j, \mathcal{M}_{(j)}, \Theta_{(j)}, r) p(\theta_j | t_j).\end{aligned}$$

Various types of proposal distribution are possible; our choice exploits the analytic results above. We take

$$q(\theta'_j, \mu'_j | \theta_j, \mu_j) \propto g(\theta'_j - \theta_j) p(\mu'_j | \theta'_j, x_j, \mathcal{M}_{(j)}, \Theta_{(j)}, r)$$

for some symmetric density  $g(\cdot)$ ; in practice we can use a suitably scaled Gaussian. Then the Hastings ratio is

$$\begin{aligned} & \frac{p(\theta'_j, \mu'_j | \mathcal{X}, \mathcal{T}, \mathcal{M}_{(j)}, \Theta_{(j)}, r) q(\theta_j, \mu_j | \theta'_j, \mu'_j)}{p(\theta_j, \mu_j | \mathcal{X}, \mathcal{T}, \mathcal{M}_{(j)}, \Theta_{(j)}, r) q(\theta'_j, \mu'_j | \theta_j, \mu_j)} \\ &= \frac{p(x_j | \theta'_j, \mathcal{M}_{(j)}, \Theta_{(j)}, r) p(t_j | \theta'_j)}{p(x_j | \theta_j, \mathcal{M}_{(j)}, \Theta_{(j)}, r) p(t_j | \theta_j)}, \end{aligned} \quad (7)$$

using the uniformity of the prior for  $\theta_j$ . The algorithm can be summarised as follows. We propose a new value for  $\theta_j$  from a symmetric distribution centred at the current value, and a new value for  $\mu_j$  from the distribution in equation 6; acceptance is based on the likelihood for  $t_j$  and  $x_j$ , as shown in equation 7. The complex dependence of  $\mu_j$  on  $\Theta$  and  $\mathcal{M}_{(j)}$  is mirrored in the proposal distribution, allowing acceptance to depend only on the likelihood.

## 6.4 Dependent calendar age errors

When we have dependence between the errors on the time axis, the algorithm of the previous section must be modified slightly. We can no longer make the simplification that  $p(\theta_j | t_j, \mathcal{M}_{(j)}, \Theta_{(j)}, r) = p(\theta_j | t_j)$ ; instead we have  $p(\theta_j | t_j, \mathcal{M}_{(j)}, \Theta_{(j)}, r) = p(\theta_j | t_j, \Theta_{(j)})$ . The simplest change is therefore to replace the Hastings ratio of equation 7 with

$$\frac{p(x_j | \theta'_j, \mathcal{M}_{(j)}, \Theta_{(j)}, r) p(\theta'_j | t_j, \Theta_{(j)})}{p(x_j | \theta_j, \mathcal{M}_{(j)}, \Theta_{(j)}, r) p(\theta_j | t_j, \Theta_{(j)})}.$$

However, there is often a parameterisation that expresses the dependence in an interpretable way. In that case, it is convenient to include such parameters explicitly. For example, if there is an error term due to the dating of a ‘floating’ chronology (Buck and Blackwell, 2004), then that will be common to all observations within that chronology. We then have

$$T_j = \theta_j + \delta_j + \omega,$$

for all  $j \in \mathcal{J}$  say, where  $\delta_j \sim N(0, \tau_j)$  and  $\omega \sim N(0, \rho)$  are all independent. We can then choose to incorporate the ‘shift’  $\omega$  in our parameterisation. We can update each  $\theta_j$  as before, with  $t_j$  replaced by  $t_j - \omega$ , and  $\omega$  itself can be updated using a simple Gibbs step, since  $p(\omega | \mathcal{X}, \mathcal{T}, \mathcal{M}, \Theta, r) = p(\omega | t_j - \theta_j : j \in \mathcal{J})$ . This does not necessarily lead to the most efficient algorithm, but it is simple to implement and to interpret; this is the approach used in the example in Section 6.5.

## 6.5 Representing the Curve

In this section, we consider briefly the use of the MCMC approach to reconstruct a part of the calibration curve. We limit ourselves to the interval 26000BP to 15000BP, to avoid the complications due to blocking alluded to in Section 6.2. The aim is simply to illustrate the process; actual updating of the curve using this approach is work in progress.

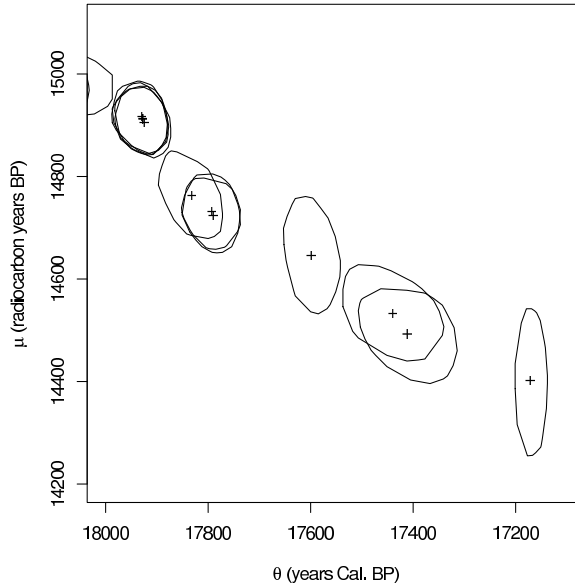


Figure 1: Posterior summaries of selected points from  $(\Theta, \mathcal{M})$

The reconstruction is based on 232 data points, with varying amounts of calendar age uncertainty. Two MCMC runs, each of 20,000 iterations with a burn-in of 5000 iterations, were used. As indicated in Section 6.1, the ‘curve’ as it would be reported consists of (a sample from) the joint posterior distribution of  $\mathcal{M}, \Theta$ . An extract from this is shown in Figure 1.

For each  $(\theta_j, \mu_j)$  an approximate 95% posterior region is given (obtained by ‘peeling’ the convex hull of the posterior sample). For example, the right-most region in Figure 1 corresponds to a data point with rather little calendar age ( $x$ -axis) uncertainty, but substantial radiocarbon age ( $y$ -axis) uncertainty. The next two overlapping regions correspond to two data-points with substantial uncertainty on both axes; the alignment of each region indicates the dependence between  $\theta_j$  and  $\mu_j$ , while the overlap on the calendar age axis indicates that we cannot be sure which of these samples is actually the older. Figure 1 does not, of course, indicate the dependence between say  $(\theta_i, \mu_i)$  and  $(\theta_j, \mu_j)$ , but that information is available in the MCMC output.

## 6.6 Calibration with MCMC

It is beyond the scope of this paper to describe in detail the various approaches that can be taken to calibration, given information on  $\mu(\cdot)$ , but it seems useful to give a brief outline of the two obvious methods. The more conservative would be to use the information on  $(\mathcal{M}, \Theta)$  to generate a conventional calibration curve i.e. means and variances at regular intervals. More natural from the Bayesian perspective however is to calibrate a point  $X_0$ , say, directly from the posterior for  $(\mathcal{M}, \Theta)$  by a further MCMC



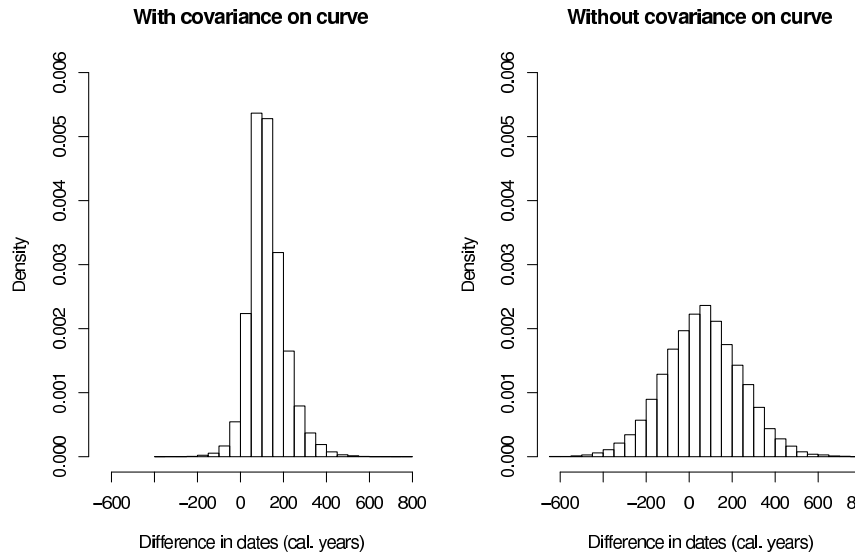


Figure 2: Posteriors for  $\theta'' - \theta'$  when  $X' = 14000 \pm 50$ ,  $X'' = 14100 \pm 50$

calculation, keeping  $(\mathcal{M}, \Theta)$  fixed but generating  $(\mu_0, \theta_0)$  just as described in Section 6.3. The latter approach makes full use of the information available, including the posterior covariance between points on the curve.

One simple example shows the potential importance of the information available from the MCMC approach but not from conventional curve construction. Imagine that we wish to make inferences about the dates  $\theta'$  and  $\theta''$  of two samples with radiocarbon determinations  $X' = 14000 \pm 50$  and  $X'' = 14100 \pm 50$ . The marginal inferences are rather insensitive to the covariance between points on the calibration curve. However, if we are interested in say  $\theta'' - \theta'$ , the covariance is crucial. Figure 2 shows the posterior distributions for  $\theta'' - \theta'$  with and without the covariance information; that is, firstly using the full information from the MCMC output, and secondly using a conventional approach to calibration that treats the reconstructed points on the calibration curve as independent. It is clear that including the covariance information substantially changes the interpretation of this result.

## 7 Discussion

By taking a Bayesian approach to radiocarbon calibration curve estimation, we have provided a methodology that takes account of sources of calendar age uncertainty that, for decades, had been ignored. We have also encouraged the radiocarbon dating community to see  $^{14}\text{C}$  variation as a process about which we have at least some prior information that should be accounted for in our curve estimation methods. Alongside this, we have built a rapport with the IntCal Working Group and are making plans to update the curve estimates again. This on-going work will be considerably enhanced by

a recent grant from the UK's Natural Environment Research Council (NERC) which will fund the provision of both MCMC methodology and user-friendly code that will be used for future updates of the calibration curves.

Other statistical aspects that we aim to investigate include the following.

- There are several aspects of calibration data collation and management that, until now, we have not had the resources to investigate, but would certainly benefit from input from statisticians. One example is that data providers currently each undertake their own “wobble matching” of floating sequences. This has meant that each match has been undertaken independently of any others and that all have been undertaken separately from curve estimation. We would like to find a way for these to be done altogether.
- There is prior information about  $\mu(\cdot)$  that we are not currently using. For example, solar cycles are known to impact the production of  $^{14}\text{C}$  and it would be interesting to investigate the impact of a component of periodic behaviour in our prior. This seems potentially important since there are cycles, with periods 11 and 25 years for example, detectable in our 2004 estimate of the curve.
- Given the results shown in Figure 2, we would like to begin to encourage the radiocarbon user community to see the calibration curve  $\mu(\cdot)$  as more than simply a collection of independent points and standard deviations, and to make appropriate allowance for its dependence structure when using it for calibration.
- Taking the previous point a step further, we would like to begin to try to convey to the user community the idea that the estimation of  $\mu(\cdot)$  and of  $\theta_0$  are not necessarily best seen as two separate steps. Almost all material sent for radiocarbon dating comes with some prior information about its calendar age, and sometimes this is quite informative. For example archaeologists often have stratigraphic information that relates the calendar dates of their samples one to another **and** they can tell us *a priori*, to the nearest 1000 years say, what period the site dates to (because culturally similar sites have been dated before). Once we combine this information with the radiocarbon data from the site in question **and** the data in the calibration database, we have the potential to learn more about the calibration curve as well as about the dates of the samples from the archaeological site. This is not something that is widely appreciated within the user community, so we will need to demonstrate the impact of doing joint inference and provide suitable software.

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