# **Deposition Models for Chronological Records**

Christopher Bronk Ramsey

Research Laboratory for Archaeology, University of Oxford, Dyson Perrins Building, South Parks Road, Oxford, OX1 3QY

#### Abstract

Long term sedimentary sequences provide a wealth of useful information for research into the palaeo-environment, especially in relation to past climate change. Shorter records provide similar information in many archaeological contexts. However if such records are to be used to provide precise timing of events, and more critically the relative timing between different records, methods are needed to provide accurate and precise age-depth models for these sequences. Given the imprecision of individual calibrated radiocarbon determinations it is necessary to use the information we have about the deposition process to refine our chronologies and also to provide interpolation between dated levels in any sequence. Even with layer counted chronologies, the uncertainties are sometimes hard to quantify.

This paper outlines a range of Bayesian models for deposition which have been implemented in the computer programme OxCal. These models can be used to combine information from the sediments themselves with radiocarbon or other direct dating information. Such models have the potential to integrate information between different records and provide a coherent chronology on which to base environmental or archaeological research.

*Key words:* Dating, Statistics, Radiocarbon, Calibration, Sedimentation, Late glacial, Quaternary environments, Ice cores, Varves

# 1 Introduction

In order to integrate the time-scales of different palaeo-climate records it is necessary that the chronologies for each record are determined with sufficient precision and accuracy. This entails the incorporation of information from a number of different sources including absolute age information, relative age information and cross correlations between records. This requires the building of some sort of model whether *ad hoc* or formal. Absolute age information can come from a variety of sources. Sometimes we have documentary information relating events to specific years; more often we have to deal with ages from scientific dating methods with their inevitable uncertainties. Relative age information likewise can be very precise as is the case for annually laminated ice cores or it can be derived from assumptions about deposition rates. When dealing with cross correlations between cores we have to be careful not to introduce circularity, for example by assuming that climatic signals are synchronous. That said, some signals (such as the primary deposition of tephra particles) are synchronous in terms of a time-scale measured in years.

If we are to achieve the required degree of precision and accuracy we need to treat the uncertainties associated with the various forms of information correctly and specifically we need to be aware when these uncertainties are correlated in some way, and when they are truly independent.

## 2 Methodological background

In order to be able to put together information of the kind that is useful in this context a mathematical framework is required. The one that is employed in this paper is the Bayesian approach which allows us to combine information of a probabilistic nature in a formal way and which has been applied in various forms in palaeo-climate records recently (e.g. see Walker et al. (2003) and Blockley et al. (2004). Bayesian methods have been applied to constrained radiocarbon dates for many years now (Buck et al. (1991), Buck et al. (1992)) and with greater frequency since the availability of software to perform such analyses (Bronk Ramsey (1995), Bronk Ramsey (2001), Jones and Nicholls (2002)). For details of Bayesian theory readers should look elsewhere (e.g. see Gilks et al. (1996), D'Agostini (2003) and particularly Buck et al. (1996) and Buck and Millard (2001)).

There are some aspects of Bayesian nomenclature which it is useful to clarify in this context. In particular, there are two terms frequently used which need to be understood. The first of these is the *prior* model. This is essentially what we know about any system before we start some set of measurements. The second is the *likelihood* which describes the information that we get from the set of measurements itself. Bayes theorem tells us how to combine these types of information. In the context of a depositional model of the type described here we will build a *prior* model which incorporates information on, for example, the order of deposition and depth information. The actual dating information can then be introduced in the form of probability distribution functions (PDFs) which represent the *likelihood* that any one sample has a particular age. What we are aiming to do mathematically is then to find a representative set of possible ages for each depth point in a sedimentary sequence. In practice, as the ages are highly correlated by depth, this is a task which is usually impossible to perform analytically and so we use a method called Markov Chain Monte Carlo (MCMC) sampling to build up a distribution of possible solutions (see Gilks et al. (1996)). Using Bayes theorem the algorithms employed essentially sample over all possible solutions with a probability which is a product of the *prior* and *likelihood* probabilities. The resulting distributions are referred to as the *posterior* probability densities and take account of both the deposition model and the actual age measurements made.

Implementation of models of this kind are too complex for most people to tackle from scratch. The models discussed here are all implemented in the software package OxCal (v4.0) which is freely available<sup>1</sup>. This program allows the information necessary for analysis to be entered and then automates the model specification and analysis stages. The full mathematical specification for the model is also given for reference. The MCMC analysis in OxCal v4.0 exclusively uses the Metropolis-Hastings algorithm (see, for example Gilks et al. (1996)) rather than the mix of Gibbs-sampling and Metropolis-Hastings used in previous versions of the program. This paper does not go into details of the MCMC implementation itself, only the formulation of the deposition models.

# 3 Deposition Models

In order to specify a deposition model completely we need to deal both with any direct dating information (referred to here using the Bayesian term *likelihood*) and the information that relates the different components of the sedimentary sequence (the *prior* model). In practice the exact dividing line between the *prior* and the *likelihood* can be arbitrary. For example it can be questioned if the information giving the local reservoir offset for a region is part of the *likelihood* or part of the *prior*. Fortunately it makes no difference mathematically to the end result though it does affect some of the diagnostic measures (such as the agreement index - see section 4.1.1).

## 3.1 Likelihoods

It is by means of the *likelihoods* that the absolute date information is entered. This information can come in a variety of forms. One of the most common is

 $<sup>^1\,</sup>$  programme available for use online at https://c14.arch.ox.ac.uk/oxcal

radiocarbon date information. This is entered into the model in the form of a calibrated date distribution (see for example Bronk Ramsey, 2001). In OxCal such a distribution can easily be entered when setting up a model with the  $R_Date$  function. So for example:

R\_Date("A",3450,28);

will indicate that an event A has a likelihood characterised by a radiocarbon date of  $3450 \pm 28$ . For the calibration of the radiocarbon date a calibration data-set is required (such as Reimer et al. (2004) or Hughen et al. (2004)) and in the case of marine samples a local  $\Delta R$  offset. For applications like this it is important that the  $\Delta R$  offset is treated as a correlated uncertainty in relation to the depositional model on all of the relevant dates (as recommended by Jones and Nicholls, 2001); this is the case in OxCal v4.0,where the  $\Delta R$  offset is treated as a model parameter with a normally distributed prior, but not in previous versions of the software.

Radiocarbon is unusual in generating such complicated likelihood distributions. For most dating methods a uniform, or normal (Gaussian) distribution can be used. The following are all allowed definitions of age likelihoods of this form:

Age(N("B",3000,30)); Age(U("C",2970,3030)); Age(Top\_Hat("D",3000,30));

the first being a normal distribution about 3000 and the next two are different ways of describing uniform distributions. The form of these distributions is shown in figure 1. We will return to examples of their use later.

# 3.2 The deposition process

Before looking at possible mathematical formulations for *prior* models of the deposition it is worth looking at the deposition process itself in some detail to see what features of real depositional systems we would like to include in our models. There are three main aspects of any deposition process which we need to take into account:

- complexity in the underlying mechanisms
- random elements to the processes
- abrupt changes to different modes of deposition

The first two of these alone might lead us to give up on producing deposition models. The third is a further complication. However, if we look at real

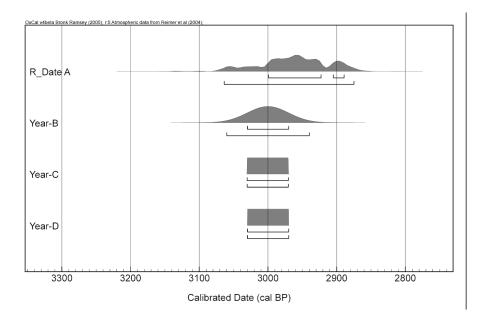


Fig. 1. Typical likelihood distributions for chronological information (see section 3.1.

sedimentary sequences a number of factors are apparent. Firstly the abrupt changes in modes of deposition are usually recognisable in terms of the sediments themselves. In other words the expertise of the sedimentologist can be used to specify these deposition boundaries and apply these as prior information in our model. In other cases such discontinuities are clearly apparent in the radiocarbon data themselves. Furthermore we know that in many cases (for example peat growth or lake sedimentation), despite the complexity and randomness of the processes, the deposition rate is approximately constant. In the end what this means is that the randomness of the process is on a sufficiently fine scale that the deposition appears continuous and uniform. Of course this is only true for as long as any one mode of deposition persists. In other cases deposition is very random and piece-wise (for example slumps, deposition from major flood events or archaeological site formation).

In some instances the actual deposition rates are known exactly. This is theoretically the case in tree-ring sequences, varved lake sediments and ice cores. Such situations can easily be dealt with a defined deposition rate (see Bronk Ramsey et al. (2001) and the  $D_{-}Sequence$  function of OxCal). An extension to this is where the deposition rate is known approximately (see the  $V_{-}Sequence$  function in OxCal Bronk Ramsey (1995)).

One more general model that has often been applied is one where the accumulation rate is unknown but assumed to be completely constant (see for example Kilian et al. (2000) or Christen et al. (1995)); in this paper this will be referred to as the uniform deposition model (or implemented as  $U\_Sequence$  in OxCal v4). Another general model is that which merely constrains the dated events to be in the order that they are within the sediment (implemented as a *Sequence* in Oxcal - Bronk Ramsey (1995)); this is applicable in cases where we can make no direct use of the depth information at all because the random nature of the deposition process is very extreme.

The uniform deposition models (constant accumulation rate) have been further elaborated by allowing a number of changes in deposition rate to be automatically located within the sequence (see Aguilar et al. (2002), Blaauw et al. (2003) and Blaauw and Christen (2005)). However this is still inherently a uniform deposition model albeit broken up into a number of sections. Others have suggested using other specific non-linear curves (as in Christen et al. (1995) and Walker et al. (2003)) to define the deposition process but these still do not take into account the random nature of the processes. Mixed effect regression has also been applied (Heegaard et al. (2005)) but this does not take into account the complexity of the radiocarbon calibration information.

An alternative approach is suggested in this paper. If we consider the deposition process as being inherently random then it would be useful to see what we expect as the functional form for deposition. In order to understand this we will consider a very simple example of water collecting in a rain gauge during a period of prolonged and fairly steady rain. Because of the finite size of the rain drops the height of water in the gauge will not rise continuously but in jumps as each drop enters the gauge. The time gap between drops arriving will also vary: this process can be described in terms of a Poisson process (that is one in which the events are essentially random). This type of age-depth model will be referred to as a  $P_Sequence$ .

Figure 2 shows how the  $P\_Sequence$  model would work in practice. The larger the increments the more variable the actual deposition is likely to be, whereas with very fine increments the deposition becomes almost constant and approximates to the constant deposition model ( $U\_Sequence$ ). The increment size for a particular model is given by a parameter k which gives the number of accumulation events per unit depth.

Table 1 gives a summary of the types of deposition model discussed here and their OxCal functions. Appendix A gives the detailed mathematical formulation of these deposition models.

# 3.3 Applicability to real situations

It is necessary to consider whether or not the  $P\_Sequence$  methodology is suitable for real depositional scenarios. In addition we need to have some way to work out what the correct choice of k (increments per unit length) is for any particular situation.

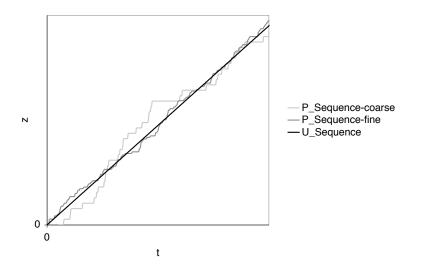


Fig. 2. Examples of deposition scenarios under three different models. In the  $U\_Sequence$  model the material builds up at a constant rate. In the  $P\_Sequence$  model there is random variation from an approximately constant rate; if the sediment is coarse (large increments, or low k parameter) the variation can be considerable; for finer sediments (small increments, or high k parameter) the accumulation is much more constant and approximates to the  $U\_Sequence$  model.

OxCal key word	Description	Equation
D_Sequence	Age gaps between points known precisely (as in	
	the case of tree rings, varved sediments or ice	A.4
	layers	
V_Sequence	Age gaps between points known approximately	A.6
	with normally distributed uncertainty	
U_Sequence	Deposition assumed to be a function of another	A.24
	parameter $z$ (usually defined as depth)	
P_Sequence	Deposition assumed to be random giving ap-	A.27
	proximate proportionality to $z$ (usually defined	
	as depth); more flexible than the U_Sequence	
	but less flexible than the Sequence	
Sequence	Ages of specified events assumed to be in the	A.22
	correct order but no use made of depth infor-	
	mation	
Table 1		

The full range of depositional models considered in this paper with their OxCal key words and equations

There may be some cases where the actual theoretical framework of random Poisson processes can really be applied. If the deposition is due to essentially random events and each deposition event is of similar size then the model can be applied directly. The k parameter is defined by the size of the deposition events. It is useful to consider such situations as they give us an idea of what a reasonable range of values might be for k. If we consider a coarse sediment containing gravel the maximum suitable value for k is likely to be around  $100 \text{ m}^{-1}$  whereas a fine sediment might well have a value of up to  $1000 \text{ m}^{-1}$ or possibly even higher. This is because of the granularity of the sediments themselves. We expect to have variability at least at the centimetre level in a gravel with grain sizes of that order whereas a much finer sediment is likely to have a more regular sedimentation, with noise on a finer scale.

In most circumstances, however, the deposition process is more complex than this. In particular, although it may be random in nature, the size of deposition events is likely to be variable and may also (as in the case of varved sediments) have a cyclical nature to it. However, in these cases the actual functional form of the  $P_{-}Sequence$  model may still be very appropriate. In section A.2.3 it can be seen that the probability distribution for an interpolated point is approximately normally distributed. Since many complex processes do lead to populations of variation with normal characteristics this leads us to expect that the functional form of the model is probably applicable in cases where the theoretical framework is not right. The difficulty in such cases is in choosing the correct parameter k.

There are cases where it might be possible to estimate an appropriate k value from direct measurements. In particular where there is an exposed section or multiple cores with stratigraphic marker layers you can use the variability in distances between the layers (see figure 3 and equation A.20). If this is not possible it may be necessary to resort to estimating k from the dating information itself (see section 4.1.2, Blockley et al. (2006b) and Blockley et al. (2006a)) but clearly this is not as satisfactory since there are dangers of circular reasoning.

As an example of another case where this model might be justified, it is also worth considering the Poisson process in relation to deposition of regular layers (such as ice or lake laminations). In such cases the deposition is usually fairly regular rather than being random. However, we can use a model like the Poisson model outlined above to deal with deviations from such a regular process. We might well expect such deviations (such as missing or double layers) to be random processes. Supposing we have a segment of sediment with m uncertain randomly disposed layers we would expect the fractional uncertainty in number of uncertain layers at the midpoint to be  $1/(2\sqrt{(m)})$ (from equation A.17) which gives an absolute uncertainty of  $\sqrt{m}/2$ . So for example an ice core or varved segment with 100 uncertain layers but with

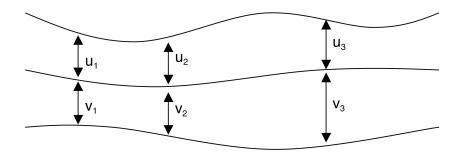


Fig. 3. Method for estimating the k parameter for exposed sections or multiple cores: three stratigraphic layers are identified and the distances  $u_i$  and  $u_i$  between them measured for each section;  $U_i = u_i/(u_i + v_i)$  and  $V_i = v_i/(u_i + v_i)$  are then calculated; from these the mean values  $\mu_U, \mu_V$  and the unbiased estimate of the standard deviation  $\sigma_U, \sigma_V$  can be calculated; for each sequence the estimate of the k parameter is then given by  $\mu_U \mu_V / [\sigma_U \sigma_V (p_i + q_i)]$  from equation A.20; for example if the three u values are measured to be 45, 50 and 48 cm and the three v values 55, 63 and 72 cm, we get estimates for k for the three sections of about 3 cm<sup>-1</sup> or 300 m<sup>-1</sup>.

a known start and end point would have an uncertainty of 5 years at the centre assuming the disposition of the errors was random. Now supposing those uncertain layers are spread over M total years. The absolute uncertainty is still the same but the fractional uncertainty is lower by a factor m/M and is equal to  $\sqrt{m}/(2M)$ ; if we use the  $P_{-}Sequence$  model defined above to model this using the layer count as the parameter z we require a k = M/m.

#### 3.4 Model definition

Appendix A covers the mathematical background to the types of depth model discussed in this paper. Here we will look at how the models can be defined in practice using the Chronological Query Language (CQL) notation of Ox-Cal (Bronk Ramsey, 1998). The definition of the three depositional models described here is performed using three functions:

- Sequence(*name*)
- P\_Sequence(*name*, k[, s])

```
P_Sequence("",1000,50)
{
 Boundary("Bottom"){};
 R_Date("",1010,25){ z=0.65; };
 R_Date("",887,25) { z=0.61; };
 R_Date("",979,25) { z=0.57; };
 R_Date("",848,25) { z=0.53; };
 R_Date("",809,25) { z=0.49; };
 Boundary("Change"){ z=0.47; };
 R_Date("",743,25) { z=0.44; };
 R_Date("",595,25) { z=0.38; };
 R_Date("",613,25) { z=0.32; };
 R_Date("",485,25) { z=0.26; };
 R_Date("",395,25) { z=0.20; };
 Boundary("Top")
                   {};
};
```

Fig. 4. Typical model specification for a short sedimentary sequence

• U\_Sequence(*name*[,s])

where *name* is the label applied to the sequence in the model, k is the assumed number of events per unit length (using the same units as for the depth z) and s is the (optional) number of automatically generated depth model points per unit length.

As an example assume that we have a sequence of 9 radiocarbon dated levels in a depositional sequence which runs from 0.675m deep up to 0.225m deep. The deposition is such that we expect the depositional unit granularity to be around a mm (or 1000 m<sup>-1</sup>). We would like to have a depth model generated at increments of about every 2cm (or 50 m<sup>-1</sup>). The sedimentology suggests that the deposition changes at a depth of 0.48m. The *P\_Sequence* model for this can then be defined as in figure 4, where the radiocarbon date for the lowest dated sample is at a depth of 0.65m and has a radiocarbon date of  $1010\pm 25$  BP and so on. The *Sequence* or *U\_Sequence* models can be defined by replacing the top line with one of:

- Sequence("")
- U\_Sequence("",50)

If the z values for the boundaries are not defined then the z is assumed to be the same as that for the next dated item in the sequence except in the case of the last boundary where it is assumed to be the same as the item just preceding it. In practice this means that for a single segment sequence the z values for the boundaries do not have to be specified unless you wish to extrapolate beyond the dated points in the sequence and only those for

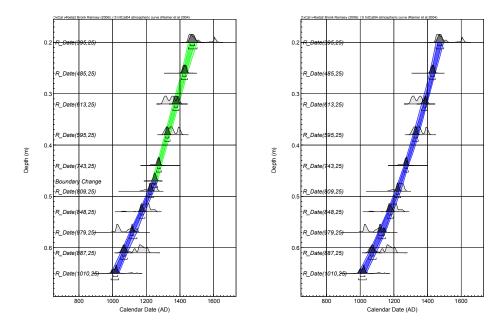


Fig. 5. This shows a depth model output for the example given in figure 4; in light grey you can see the distributions for the single calibrated dates (the likelihoods); in darker grey, the marginal posterior distributions are shown which take into account the depth model; the depth model curves are envelopes for the 95% and 68% HPD ranges; the left hand plot shows the model based on a step change in deposition rate exactly as defined in figure 4, and the right hand model that is based on an exponential rise in deposition over time (as described in section A.4.3); in this instance both models give very similar results

changes in deposition need to be specified.

In these models the underlying assumption is that the probability of deposition is constant over time. We can assume that the deposition rate is linearly rising in any segment by replacing the first Boundary with a Zero\_Boundary or for exponential rises with a Tau\_Boundary. See section A.4 for more details.

Having defined the model in this way, the OxCal program will then calculate the mathematical functions to be applied to give the appropriate prior, as outlined in Appendix A. The MCMC analysis is performed automatically to generate the posterior probability distributions for each event. The highest probability density (HPD) range is also calculated and presented in a table and can be plotted as an age-depth model (as shown in figure 5 for the example specified in figure 4).

# 4 Applications

Having defined the way in which these deposition models can be specified it is worth looking at their application in practice. In this context we will look at two specific examples.

The first example to be considered is a the varved lake sediment from Soppensee (Hajdas et al. (1993) and Hajdas et al. (2000)). This is an interesting example because it shows that the approaches outlined here can be applied both in terms of depth and in terms of varve count. The second example, is that of ice-core layer counting which is clearly critical to the work of integration of climate records.

# 4.1 Lake sediment deposition

The example of Soppensee (Hajdas et al., 1993) is chosen here because it has a number of interesting features:

- there is a good sequence of radiocarbon dates
- the sediment is varved through much of the sequence
- there are clearly some discrepancies between the radiocarbon and varve chronologies
- the Laacher See Tephra (LST) is present in the record giving some independent check of the chronology
- the chronology of the sequence has interesting implications for the timing of climatic events in the Last Glacial Interglacial Transition.

In this paper the formulation of the model for the sequence will be discussed in detail. Another paper in this volume (Blockley et al., 2006b) covers the implications of the derived chronology.

# 4.1.1 Identification of outliers

In dealing with a real example like this, the problems associated with any sedimentary sequence become immediately apparent. The first of these is the fact that there are clearly some outliers in the sequence. There are different approaches that can be used for identifying outliers. Some statisticians recommend the use of automatic outlier detection (Christen, 1994). This approach is statistically sound but it does have some difficulties. The method involves the assignment of a prior probability for any sample being an outlier and the analysis then allows samples to be down-weighted if need be. The results of the analysis depend on the outlier probability - and this is clearly very difficult

to determine in any real situation. The approach also automates an operation that perhaps ought to have some expert judgement applied to it. In some sediments, for example intrusive material (younger than context) is less likely to be present than residual material (older than context). The other approach is to identify outliers either by eye (where they are obvious) or using statistical measures but always mediated by a knowledge of the sedimentary processes. The final model is then based on a specific subset of the results and so it is clearer what information has been used to arrive at the final results. It is often useful to see how robust the results are to the inclusion or exclusion of particular key measurements.

Another method is to look for cases where the *posterior* probability distribution has a very small overlap with the *likelihood* probability distribution. In OxCal such an overlap is calculated in the form of the agreement index (Bronk Ramsey (1995)) which gives the relative likelihood of the posterior from the model to that of a 'null' model (where there are no constraints or interrelationships between the events). See chapter 9 of Gilks et al. (1996) for a discussion of these types of measure. The threshold for acceptable agreement index is 60%. This level has been chosen by empirical comparison to  $\chi^2$ tests and is criticised by some Bayesian statisticians as being arbitrary. In the end the choice is between an arbitrary prior probability for a sample being an outlier or an arbitrary cut-off in acceptable overlap between the posterior and the likelihood; there is no totally satisfactory solution. In this paper the agreement index method has been employed as this is what is implemented in OxCal. The relationship between the practicalities of rejecting dates using this threshold and the fitting of different deposition models is discussed in Blockley et al. (2006b).

Further ideas of how outliers might be treated are discussed in section 5.

In this illustrative case we wish to look at a variety of different models. So in deciding which samples to exclude from the analysis we selected those which were inconsistent with the other dates in most of the models (including the straightforward *Sequence*). This meant that there were still measurements included which were inconsistent with an entirely uniform deposition rate (using either varve count or depth).

In the end, in addition to the outliers already identified by Hajdas et al. (1993), further data-points were rejected on the basis that they gave low agreement with the selected models (Blockley et al., 2006b).

# 4.1.2 Construction of models

Because this study was drawing on already published material it was thought most appropriate to use the different sedimentary units (I to VI) of the deposit defined by Hajdas et al. (1993).

Having defined the data points to be included in the model and the boundaries, all that remains is to select the mathematical model to be employed. One possibility here would be to use the exact age differences from the varve counting to define the relative age of the samples using the known age gaps and either a  $D_Sequence$  or a  $V_Sequence$ , (see section A.1) however this presupposes that the uncertainties in the varve counting are either non-existent or very well characterised - and certainly earlier in the sequence this is clearly not the case.

Instead five different models were looked at. The first of these was simply to use the order of deposition to constrain the dates in a *Sequence*. This is the most conservative of the models and almost certainly gives much wider ranges than are realistic as neither the depth information nor the varve counts were used. However even this model gives results which are more precise than the calibrated dates alone.

The next two models assume uniform deposition  $(U\_Sequence)$  either by depth or in terms of varve count. The meaning of these is fairly clear: in the case of depth we assume that within each segment the same depth of sediment is laid down per unit time; in the case of varves we assume now, not that the varves are necessarily annual but that the number counted will be proportional to the time gap between any two points on the core. Such models are almost certainly too prescriptive since they allow for no fluctuations in deposition from year to year and they do not take into account that uncertainty in varves is likely to be due to the occasional missing or double varve in an otherwise annual sequence.

The final two models use the  $P\_Sequence$  methodology outlined above for either deposition against depth or against varve number. The problem in such cases is the estimation of the k parameter to obtain a suitable degree of flexibility for the models. The k parameter for depth was chosen to be  $300m^{-1}$  or  $3cm^{-1}$  which implies a depositional unit of about 3mm (see fig 6). For varves the k parameter was chosen to be 0.25 which implies a depositional unit of four varves (or on average about 2mm). These were the highest k which gave a satisfactory agreement with the actual dating information (using the agreement indices). This is not a very satisfactory method of choosing this parameter since it relies on the dating information being able to discriminate between different models and there is a danger of circular arguments. For example two dates will always be consistent with a completely uniform deposition - even though this might be far from the truth.

It is worth looking at the implied uncertainty in these prior  $P\_Sequence \mod$  els to see what they mean in practice. For the depth sequence model, if we had

```
P_Sequence("",3)
{
 Boundary("VI/VII"){};
 R_Date("ETH-6809",12150,90){ z=633.5; };
 R_Date("ETH-6808",11930,90){ z=631.5; };
 R_Date("ETH-6807",12040,90){ z=629.5; };
 R_Date("ETH-6806",11385,90){ z=611; };
 R_Date("ETH-6805",11300,85){ z=610; };
 R_Date("ETH-5305", 11380, 105){ z=607; };
 R_Date("ETH-6933",11470,70){ z=606; };
 R_Date("ETH-6932",11160,60){ z=600.5; };
 Boundary("V/VI"){ z=597; };
 Event("LST"){ z=595; };
 R_Date("ETH-5290",10760,105){ z=594; };
 R_Date("ETH-7703",10440,100){ z=577; };
 Boundary("IV/V"){ z=571.5; };
 R_Date("ETH-6929",10400,70){ z=569; };
 R_Date("ETH-6803",9965,75){ z=550.5; };
 R_Date("ETH-7710",10135,100){ z=547; };
 R_Date("ETH-7701",9970,100){ z=542.5; };
 Boundary("III/IV"){ z=539.5; };
 Boundary("II/I"){ z=524.5; };
 R_Date("ETH-6623",9595,70){ z=524.5; };
 R_Date("ETH-6622",9625,65){ z=523.5; };
 R_Date("ETH-7700",9530,95){ z=519.5; };
 . . .
 R_Date("ETH-7211",6325,50){ z=398.5; };
 R_Date("ETH-7353",6180,55){ z=391.5; };
 R_Date("ETH-7210/7352",6190,40){ z=390.5; };
 Boundary(){};
};
```

Fig. 6. Main elements of the model specification for the analysis of Soppensee for the case of a  $P\_Sequence$  model applied against depth; there is a long sequence of radiocarbon dates between depths of 519.5 and 398.5 cm deep not shown here (marked with ...).

a 1m segment with the age known at both ends the fractional age uncertainty (from equation A.17) at the centre would be  $1/(2\sqrt{300})$  which is 2.9% or about 60 years (assuming an average deposition per year of about 0.5mm). For the varve depth sequence, for 2000 varves (about 1m) the relative age uncertainty at the centre of a segment would be  $1/(2\sqrt{0.25 \times 2000})$  which is about 2.2% or about 45 years. In practice a better approach for an *ab initio* study might be to estimate these uncertainties directly by making a detailed analysis of part of the core or multiple cores as shown in figure 3. It is also hoped that,

with experience of using such models, better methods for estimating k from a knowledge of the sediments will be developed. It is also interesting to note that the value found empirically for this depth sequence is right in the middle of the expected range of  $100-1000m^{-1}$  (see section 3.3).

# 4.1.3 Analysis results

A typical depth model output is shown in figure 7. Here you can see how the analysis allows the depth model to be slightly non-linear even in the top section (I) and allows changes in deposition rates at boundaries. The results from the analysis of the Soppensee core are discussed in much more detail in Blockley et al. (2006b). However there are several useful lessons that can be extracted.

- the  $U\_Sequence$  models diverge slightly and show poor agreement with the actual dating information unless more outliers are rejected
- the results of both *P\_Sequence* models are very close and allow much more of the dates to be included in the model (as restricted by the *agreement index*).
- the precision of the  $P\_Sequence$  models is close to that of the varve counting precision and not much lower than the (artificially high) precision of the  $U\_Sequence$  models
- the *Sequence* model is much less precise but overlaps all of the others
- as far as we can tell the *P\_Sequence* models are accurate in their estimation of the date of the Laacher See Tephra

# 4.2 Ice core layers

Finally we come to consider, in a more speculative way, the application of the methodology outlined here to other sorts of records, which have little to do with radiocarbon calibration. In particular we will look at the way the  $P\_Sequence$  model might be applied to the estimation of interpolation and extrapolation of uncertainties in ice-core sequences.

In principle, or course, the annual layers laid down in ice cores allow the direct counting of years back from some known date. However, in practice there are errors in any such counting process. This is at least in part due to layers that are difficult to distinguish and so have to be identified as uncertain layers in the sequence. There are also other possible problems such as missing core segments, ablation events or other re-workings of the primary deposition of the ice but these are usually discussed and accounted for in initial counting of ice core layers. Here we will concentrate on the random errors associated

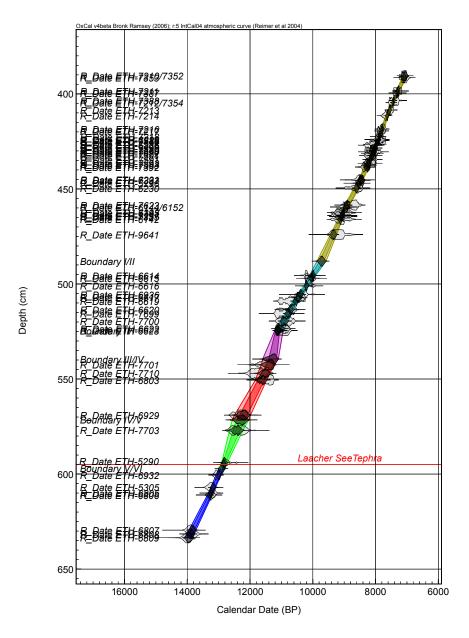


Fig. 7. Age-depth model for Soppensee using depth as the variable and assuming the deposition is a Poisson process ( $P\_Sequence$ ); the input for this model is shown in figure 6

with uncertain layers which are harder to test for using physical analyses of ice cores.

### 4.2.1 Binomial treatment

Appendix B gives a simple Binomial treatment of ice-core uncertainties. In this we assume that each uncertain layer has a probability of 0.5 of being real and 0.5 of being illusory. If, for example, there are a total of N = 1600 uncertain layers (as determined by the analysis of the original ice core layer count) the most likely number of true layers amongst these is N/2 = 800 and the 95% confidence range is  $\pm \sqrt{N} = \pm 40$ . From this it can be seen that for a core with a total of N = 1600 uncertain layers and 39200 definite layers the 95% range would be  $40000 \pm 40$  which is compared to the 100% range of  $40000 \pm 800$ .

However, this simplified treatment has some problems associated with it. Most critically, we do not know that the probability of an uncertain layer being real is exactly 0.5, it might in fact be 0.9 or 0.1, and clearly our lack of knowledge of this probability far outweighs the uncertainty estimated from this type of analysis.

# 4.2.2 P\_Sequence treatment

Instead of the Binomial treatment we wish to consider the problem using a  $P\_Sequence$  model against layer count. We will again assume, for the sake of argument, that within a 40000 year sequence there are 1600 uncertain layers. We can (other possible problems aside) then use these uncertainties to define a maximum range of possible dates for each depth within the sequence. So at 40000 layer counted ice core years, we know that the true age lies between 39200 and 40800 - and we will assume that any of these ages is equally likely. Such a distribution can be defined in OxCal using the  $Top\_Hat$  function as Age(Top\\_Hat(40000,800)). We will then also use the result we derived in section 3.3 that for m uncertain layers in a total of M, a suitable k for a  $P\_Sequence$  is equal to M/m which in this case gives k = 25. We can then build a model for the sequence as a whole.

Figure 8 shows two possible such models. The first model (I) assumes that we know no more than this about the date of layers within the core. The top of the core is fixed within a year. If we then look at the output from the deepest point which is shown as A1 in figure 9 we can see that the posterior distribution is very little altered by the model. This makes sense as although the distribution is forced to be fairly uniform with respect to layer count the uncertain layers can, in principle all be real or all false. However, model II shows that if, for example, we have a well dated event for the 10000'th layer which is 10000  $\pm$ 10 years old (with normally distributed errors), the model becomes much tighter giving us a 95% HPD range of some 320 years at the earliest point in the sequence. This is much more realistic than the 80 year range from the Binomial treatment. Whether it is accurate or not in a particular instance is hard to ascertain. This is because there may by systematic effects that have not been taken into account. We assume here that the error rate is independent of depth which is probably not reasonable. It may therefore, in a real case, be necessary to split the sequence into segments with similar characteristics.

```
P_Sequence("Model I",25)
{
 Boundary(){};
 A1=Age(Top_Hat(40000,800)){ z=40000; };
 B1=Age(Top_Hat(30000,600)){ z=30000; };
 C1=Age(Top_Hat(20000,400)){ z=20000; };
 D1=Age(Top_Hat(10000,200)){ z=10000; };
 E1=Age(N(0,1))
                           { z=0; };
 Boundary(){};
};
P_Sequence("Model II",25)
{
Boundary(){};
 A2=Age(Top_Hat(40000,800)){ z=40000; };
 B2=Age(Top_Hat(30000,600)){ z=30000; };
 C2=Age(Top_Hat(20000,400)){ z=20000; };
D2=Age(N(10000,10))
                          { z=10000; };
                           { z=0; };
 E2=Age(N(0,1))
Boundary(){};
};
```

Fig. 8. Two model definitions for ice core sequences; in model I only the layer counting uncertainties are included; in model II a well dated event has been introduced at 10000 years ago.

However, in cases where we have multiple cores and multiple tie points, all of this information can, at least in principle, also be built into the model and we have the potential to construct a truly integrated chronology although, in the case of Greenland, this would involve some assumptions about time transgressions.

# 5 Further developments in modelling deposition processes

It is certainly possible to further refine these models and a few possibilities will be discussed here. However, it should always be remembered that further complexity comes at a cost - both in terms of analysis time and, more importantly, in terms of clarity. No model will fully encapsulate all of the details of the real processes and it may be better to keep the model sufficiently simple that it is relatively easy for the informed user to intuitively understand the assumptions underlying it.

The first area where we might wish to add extra aspects to the model is to deal with dated samples that are not exactly the same age as the deposits in which

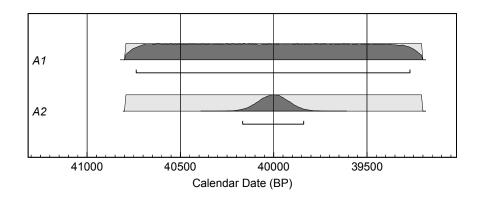


Fig. 9. Output from the models defined in figure 8; A1 gives the distribution for the start of the sequence assuming only the ice layer information; in light grey is the traditional maximum error estimate and in dark grey the results of the Bayesian analysis showing very little change; A2 shows the result of including an age constraint at 10000 years ago on the estimate for the date of the start of the core; in both cases the 95% HPD range is shown.

they are found. There are various different ways in which such samples can be treated. Above (section 4.1.1) we looked at the treatment of some results as outliers, either identified by the user, or by the use of automatic outlier detection.

One possible elaboration of the models described here would be to add the automatic outlier detection methods developed by Christen (1994). However a different approach has been taken in OxCal v4. This allows any date to be offset by some unknown amount - we can then model the offsets for a whole sedimentary sequence in a number of different ways:

- The most straight-forward is simply to assume that they are part of a normal distribution of unknown variance; the analysis will then find that variance while constraining the mean to be zero (that is the dates are assumed to be on average correct). Although this is simple it perhaps shares some of the same problems of the automatic outlier detection in that if the reasons for offsets are not understood, we cannot be sure that they average to zero. However it might be applicable in cases of bi-directional bioturbation. This approach was tested in Blockley et al. (2006a).
- The other two distributions of offsets that can be modelled are suited to the situation where we know that the samples are suspected of being residual (older than their context) or intrusive (younger than their context). In these cases we can assume that they are distributed as an exponential tail either to the older or younger side of the sequence. Again the analysis can determine the time constant of this exponential tail.

These methods of dealing with offsets would seem to offer a reasonable description of what is going in the depositional processes. Other information might also be brought into a model using additional parameters. For example, in the example outlined in Figure 4 we might have information about the relative duration of both segments of the deposition. In OxCal we can apply a prior probability distribution to the ratio of these durations. This is done by adding the following two lines to the model definition:

Ratio=(Top-Change)/(Change-Bottom); Ratio&=N(1.0,0.1);

The first of these lines defines another parameter 'Ratio' which is the ratio of the duration of the upper segment to that of the lower segment; the second line then assigns a prior probability to this ratio which is a normal distribution with a mean of 1.0 and a standard deviation of 0.1. In principle any functional form can be given to this prior. The ability to add such information is potentially useful, however in practice it is rare that such information is know in quantitative form.

Two other developments are possible, although they have not yet been implemented. The first is to allow for the actual depth of a sample in a sediment to be uncertain - effectively an alternative to dealing with any offsets in the time dimension. The second, which is more difficult, is to make the k parameter of the *P\_Sequence* model a variable - so that the analysis can find the most appropriate value automatically. This is attractive given the difficulty in assessing a suitable value. That said, there are some disadvantages in such an approach:

- a suitable prior distribution for k would have to be defined anyway
- the value of k would become strongly dependent on the treatment of offsets or outliers since if the offsets are large enough any distribution could be fitted to a straight line
- the resultant model output would be dependent on a series of assumptions that it is hard to comprehend easily and perhaps equally hard to justify.

So although further mathematical elaborations of the models are theoretically possible, these should not be expected to solve all of the problems in dealing with depositional models. Ultimately if you have a number of offset dates whose cause and distribution is hard to ascertain and you also do not know how regular your deposition is, you do not have enough information to produce a good age depth model and no statistical sleight of hand is going to help with this.

As discussed in Blockley et al. (2006b) modelling needs to be combined with other stratigraphical information and laboratory analyses. However, when this is achieved, robust high precision age models can be produced.

# 6 Conclusions

In this paper a number of different depth models have been discussed. These come into two broad categories: the specific models for use in instances where the deposition rate is known either precisely ( $D\_Sequence$ ) or approximately ( $V\_Sequence$ ) and the more general models where the actual deposition rate is unknown.

The generalised models cover a whole spectrum from those where the deposition is assumed to be exactly uniform ( $U\_Sequence$ ) through to cases where all we can say is that the deposition took place in a particular order (Sequence). The  $P\_Sequence$  fills this spectrum with a k parameter defining the stiffness of the model; if k = 0 this gives a model identical to a Sequence and if  $k = \infty$  (infinity) the model is the same as a  $U\_Sequence$ . From a theoretical perspective the  $P\_Sequence$  would seem to be the most realistic in all real cases since no deposition is truly uniform and neither is it such that the depth can tell us nothing (as in the case of the Sequence).

In support of this, all of the deposition models discussed here have been assessed on synthetic sedimentary sequences and the  $P\_Sequence$  found to be the most effective, in general terms, at reproducing the true sedimentation rate in all cases considered (Blockley et al., 2006a).

The implementation of these models in OxCal, allows us to produce age-depth models for a whole range of chronological records. It also, equally importantly, allows us to study the sedimentation process to better understand issues such as residuality, intrusion and changes in sedimentation rate.

# 7 Acknowledgements

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### APPENDICES

#### A Mathematical formulation of deposition models

This section will deal with the mathematical formalism that underlies the deposition models defined in this paper. The aim is to model the deposition events that led the record as it is currently found. The events are labelled from the start (bottom) of the record i = a to the end (top) i = b. They are assumed to have occurred at times  $t_i$  (which are calendar dates and not to be confused with the radiocarbon dates) and to correspond to specific depths  $z_i$  in the record. In some models the actual depths are not used but in all cases we assume that the events occurred in a specific order - that is that:

$$t_i < t_{i+1}$$
 for all *i* such that  $a \le i < b$  (A.1)

This can be expressed in terms of an unnormalised prior which is defined as:

$$p_H(\mathbf{t}) = p_H(t_a, t_{a+1}, \cdots, t_b) = \begin{cases} 1 & t_a < t_{a+1} < \cdots < t_b \\ 0 & \text{otherwise} \end{cases}$$
(A.2)

We will also assume that z changes monotonically with time. For clarity we assume that z increases with increasing t:

$$z_i < z_{i+1}$$
 for all *i* such that  $a \le i < b$  (A.3)

although z could equally well be defined to be depth below the surface without affecting the models (the OxCal implementation will accept z as height or depth). The overall model can usefully be split into three main components:

- the likelihood distributions  $p(y_i|t_i)$  for individual parameters (see section 3.1) where, for example, direct dating information  $y_i$  is included for a specific date  $t_i$ . The product of all of these will be denoted by  $p(\mathbf{y}|\mathbf{t}) = \prod_i p(y_i|t_i)$ .
- the constraints on the parameters (in the case of sedimentary sequences these are given in equation A.1 or, as a prior, in equation A.2)
- other informed prior probability functions relating the specific parameters (which are described in this section)

In all cases we will assume that the uninformed prior for any parameter  $p(t_i)$  is constant. Their product  $p(\mathbf{t})$  will therefore also be constant.

#### A.1 Known age gaps

Before discussing generalised deposition models it is worth considering a couple of special cases. The first of these is the case where the exact time interval is known between two different points in the deposition sequence. This is theoretically the situation with a varved sediment or a tree ring sequence. In such cases we have information which defines the time gap precisely (referred to here as a  $D_{-}Sequence$ . We have:

$$t_{i+1} = t_i + g_i$$
 for all *i* such that  $a \le i < b$  (A.4)

where  $g_i$  is the gap between one point and the next. In practice such a model has only one independent variable (which can be chosen to be the start of the sequence,  $t_a$ ) since all of the relative ages are exactly defined. This type of model is already widely used (see Bronk Ramsey et al. (2001) and Christen (2003)). If we take the prior for  $t_a$  to be uniform the posterior is proportional to the product of the likelihoods with **t** being a a function only of  $t_a$  and **g**:

$$p(\mathbf{t}|\mathbf{y}, \mathbf{g}) \propto p(\mathbf{y}|\mathbf{t}(t_a, \mathbf{g}))$$
 (A.5)

Some allowance for variation can be introduced where this gap is only approximately known with a mean gap of  $g_i$  and an uncertainty in that figure of  $s_i$ . Then we have:

$$t_{i+1} = t_i + g_i \pm s_i$$

$$p(t_i, t_{i+1}|g_i, s_i) \propto \frac{1}{s_i \sqrt{2\pi}} \exp\left(-\frac{(t_{i+1} - t_i - g_i)^2}{2s_i^2}\right)$$

and the informed prior probability contains a factor proportional to:

$$p(\mathbf{t}|\mathbf{g},\mathbf{s}) \propto \prod_{i=a}^{b-1} \frac{1}{s_i \sqrt{2\pi}} \exp\left(-\frac{(t_{i+1} - t_i - g_i)^2}{2s_i^2}\right)$$
 (A.6)

Using Bayes theorem, the posterior probability then becomes:

$$p(\mathbf{t}|\mathbf{y}, \mathbf{g}, \mathbf{s}) \propto p(\mathbf{y}|\mathbf{t})p(\mathbf{t}|\mathbf{g}, \mathbf{s})p_H(\mathbf{t})$$
 (A.7)

Such models have been implemented in OxCal (Bronk Ramsey, 1995) as a  $V\_Sequence$ . These models do not use depth information at all explicitly, except in as much as they are subject to the constraint given in equation A.1 and can only be used for age-depth models in very particular circumstances. Other

functional forms might be more appropriate and this can also be catered for. The usual way of doing this is to define parameters for the intervals between events  $d_i = t_{i+1} - t_i$  and then assign a likelihood function to the parameter  $d_i$ . This additional information can be used to further constrain the Sequence model described in the following section.

#### A.2 Interpolation between points

In order to make use of depth information we need some method of interpolation between points of known age. Let us suppose that we know the (calendar age) time  $t_i$  of depth  $z_i$  and the time  $t_{i+1}$  of depth  $z_{i+1}$ . What we would like to know is what the probability distribution function is for the time t at depth z such that  $z_i < z < z_{i+1}$  (and thus  $t_i < t < t_{i+1}$ ).

#### A.2.1 Simple ordered deposition (Sequence)

Consider the case of the model in which all we assume is that the deposition is monotonic (which in a sedimentary sequence simply means that there are no erosional episodes). This model will be referred to here as a *Sequence*. In this case for any intermediate depth all we know is that the time of deposition must lie somewhere between  $t_i$  and  $t_{i+1}$ . In this case there is a uniform prior for t over the range  $t_i$  to  $t_{i+1}$ :

$$p(t|z) = \begin{cases} \frac{1}{t_{i+1}-t_i} & t_i < t < t_{i+1} \\ 0 & \text{otherwise} \end{cases}$$
(A.8)

#### A.2.2 Uniform deposition ( $U\_Sequence$ )

Next let us consider the model of uniform deposition that is often applied (see example 2 in Christen et al. (1995) or see Kilian et al. (2000)). In this model (*U\_Sequence*) the time at any particular depth is exactly defined through linear interpolation over the range  $z_i \leq z \leq z_{i+1}$ :

$$t = t_i + (t_{i+1} - t_i) \frac{(z - z_i)}{(z_{i+1} - z_i)}$$
(A.9)

#### A.2.3 Poisson model deposition (P\_Sequence)

Finally we turn to the Poisson mediated deposition model ( $P\_Sequence$ ). In this case to derive a probability distribution we need to know the size of the incremental jumps in depth. In the case of the rain analogy this is the height gain in the rain gauge due to one rain drop, with every drop having the same size. We will introduce this as a parameter k which is the number of increments per unit length - so if it takes 1000 rain drops to raise the level in the gauge by 0.01 m then  $k = 10^5 \text{m}^{-1}$ . The total number of increments occurring in the range  $z_i$  to  $z_{i+1}$  is then simply  $N = k(z_{i+1} - z_i)$  and the number arriving in the range  $z_i$  to z is  $n = k(z - z_i)$ . Strictly speaking N and n should be integers since z is only able to change by increments of 1/k. The arrival times of the N increments are assumed to form a Poisson process, with exponentially distributed intervals between arrivals, and with an unknown but constant arrival rate.

The arrival time of each increment has a uniform probability distribution function:

$$f(t') = \begin{cases} \frac{1}{(t_{i+1}-t_i)} & t_i < t' < t_{i+1} \\ 0 & \text{otherwise} \end{cases}$$
(A.10)

and therefore the probability that any such increment takes place between  $t_i$  and t is:

$$q = \int_{t_i}^t f(t')dt' = \left(\frac{t - t_i}{t_{i+1} - t_i}\right)$$
(A.11)

Thus the probability that n of them precede t and N - n succeed t is given by:

$$p(n|t, N) \propto \frac{N!}{n!(N-n)!} \left(\frac{t-t_i}{t_{i+1}-t_i}\right)^n \left(\frac{t_{i+1}-t}{t_{i+1}-t_i}\right)^{N-n}$$

$$= {}_N C_n q^n (1-q)^{N-n}$$
(A.12)
$$\approx \frac{1}{n!(N-n)!} \exp\left(-\frac{(n-Nq)^2}{n!(N-n)!}\right) \quad \text{for large } N \quad (A.13)$$

$$\approx \frac{1}{\sqrt{2\pi Nq(1-q)}} \exp\left(-\frac{(n-Nq)^2}{2Nq(1-q)}\right) \qquad \text{for large } N \quad (A.13)$$

which is a likelihood function for n. We now use Bayes theorem, observing that  ${}_{N}C_{n}$  is independent of t and assuming that the uninformed prior p(t) is uniform. From equation A.12 we find an informed prior for t:

$$p(t|n, N) \propto p(n|t, N)p(t)$$

$$\propto q^{n}(1-q)^{N-n}$$

$$p(t|z, k) \propto \frac{(t-t_{i})^{k(z-z_{i})}(t_{i+1}-t)^{k(z_{i+1}-z)}}{(t_{i+1}-t_{i})^{k(z_{i+1}-z_{i})}}$$
(A.14)

By taking the derivative of equation A.14 (with regard to t) and equating to zero we see that this function reaches a maximum when:

$$\frac{z - z_i}{t - t_i} = \frac{z_{i+1} - z}{t_{i+1} - t} \tag{A.15}$$

which makes sense as this is equal to the interpolated point from the  $U_Sequence$  (since equation A.15 can be rearranged to give equation A.9). If we now assume that N is large and that we are close to this maximum the distribution p(t|z, k) approximates to a normal distribution with respect to t with a mean:

$$\mu_t = t_i + (z - z_i) \left( \frac{t_{i+1} - t_i}{z_{i+1} - z_i} \right)$$

and a standard deviation of:

$$\sigma_t = (t_{i+1} - t_i) \sqrt{\frac{(z - z_i)(z_{i+1} - z)}{(z_{i+1} - z_i)^2}} \frac{1}{\sqrt{k(z_{i+1} - z_i)}}$$
(A.16)

This is useful as it allows us to see the effect of different k parameters on the rigidity of the depth model. In particular we can see that for a midpoint the fractional uncertainty  $\sigma_t/(t_{i+1} - t_i)$  is:

$$\frac{\sigma_t}{(t_{i+1} - t_i)} = \frac{1}{2} \frac{1}{\sqrt{k(z_{i+1} - z_i)}} = \frac{1}{2} \frac{1}{\sqrt{N}}$$
(A.17)

More generally we can estimate k where we have some measure of the variability of the sedimentation rate in different sections. We are most likely to know how variable z is for some specific t. We can use equation A.13, and the assumption that we are not too far from the maximum probability, to estimate the expected standard deviation in z:

$$\sigma_{z} = \frac{\sigma_{n}}{k} = \frac{1}{k} \sqrt{Nq(1-q)}$$

$$= \frac{\sqrt{N}}{k} \sqrt{\frac{(t-t_{i})(t_{i+1}-t_{i})}{(t_{i+1}-t_{i})^{2}}}$$

$$\approx \frac{\sqrt{N}}{k} \sqrt{\frac{(z-z_{i})(z_{i+1}-z_{i})}{(z_{i+1}-z_{i})^{2}}}$$

$$\frac{\sigma_{z}}{(z_{i+1}-z_{i})} \approx \sqrt{\frac{(z-z_{i})(z_{i+1}-z_{i})}{(z_{i+1}-z_{i})^{2}}} \frac{1}{\sqrt{N}}$$
(A.18)

We can make measurements that allow us to estimate this if we have multiple cores sharing chrono-stratigraphic markers or an exposure with identifiable layers. Let us define:

$$u = z_{i+1} - z$$

$$v = z - z_i$$

$$U = u/(u + v)$$

$$V = v/(u + v)$$
(A.19)

By measuring u and v in several places (see figure 3 in the main text) we can find mean and standard deviations for U and V (the means being defined as  $\mu_U, \mu_V$  and the standard deviations as  $\sigma_U, \sigma_V$ ). We then have from equation A.18:

$$\sigma_U = \sigma_V \approx \frac{\sigma_z}{(z_{i+1} - z_i)}$$
$$= \sqrt{UV} \frac{1}{\sqrt{N}}$$
$$\sigma_U \sigma_V \approx \mu_U \mu_V \frac{1}{N}$$
$$N \approx \frac{\mu_U \mu_V}{\sigma_U \sigma_V}$$

And then for each sedimentary sequence we arrive at an estimate for the k parameter,  $k_{est}$ :

$$k_{est} = \frac{\mu_U \mu_V}{\sigma_U \sigma_V} \frac{1}{(u+v)} \tag{A.20}$$

To summarise the nature of interpolation using this  $P\_Sequence \mod l$ : the probability peaks at the same point as that derived from the  $U\_Sequence \mod l$  and, like the Sequence model, falls to zero as t approaches either  $t_i$  or  $t_{i+1}$ . As k tends to zero the distribution becomes identical to the Sequence model and as it tends to infinity it effectively becomes the same as the  $U\_Sequence \mod l$ . At intermediate values where k is high the distribution becomes very similar to a normal (Gaussian) distribution.

#### A.3 Overall prior probabilities

Let us now set up the entire prior probability associated with the three generalised models under consideration here (Sequence,  $U\_Sequence$  and  $P\_Sequence$ ) and see how they might be used to calculate posterior probability densities. In all cases we will consider the sedimentary sequence in sections which are defined by *boundaries*. These sections can essentially be treated independently although there may be some constraints, such as the start of one section being of the same age as the end of the previous one.

For each segment of interest we have the event a (at time  $t_a$ ) which is the start of the segment, an event b (at time  $t_b$ ) which marks the end of the segment, and all of the intermediate events of interest  $a + 1 \cdots b - 1$  (at times  $t_{a+1} \cdots t_{b-1}$ ). Within the segment we assume that the deposition process remains the same and that we have the constraints  $t_i < t_{i+1}$  (and thus  $t_a < t_b$ ).

## A.3.1 Simple ordered deposition (Sequence)

In the case of the simple *Sequence*, the prior probability density for any single event  $t_{a+1} \cdots t_{b-1}$  occurring at time t' is given by:

$$f_u(t') = \begin{cases} \frac{1}{(t_b - t_a)} & t_a < t' < t_b \\ 0 & \text{otherwise} \end{cases}$$
(A.21)

And choosing the prior for  $t_a$  and  $t_b$  to be uniform, the overall informed prior probability, subject to the constraints given in equation A.1, is proportional to:

$$p_u(\mathbf{t}) \propto \prod_{i=a+1}^{b-1} \frac{1}{t_b - t_a} = \frac{1}{(t_b - t_a)^{b-a-2}}$$
 (A.22)

and as the total number of possible combinations of  $t_i$  is proportional to  $(t_b - t_a)^{b-a-2}$  this prior is neutral with respect to the length of the segment. The posterior is then calculated as:

$$p_u(\mathbf{t}|\mathbf{y}) \propto p(\mathbf{y}|\mathbf{t})p_u(\mathbf{t})p_H(\mathbf{t})$$
 (A.23)

In OxCal such a model would be defined using the commands:

```
Sequence()
{
  Boundary("a");
  ...
  Boundary("b");
};
```

#### A.3.2 Uniform deposition ( $U_{-}Sequence$ )

In the case of the uniform sequence, or  $U\_Sequence$ , the deposition rate is assumed to be exactly defined by:

$$\frac{dz}{dt} \propto f_u(t) = \text{constant}$$
 within the range  $t_a < t < t_b$ 

And so integrating with respect to time, and choosing  $t_a$  and  $t_b$  to be our independent variables with uniform priors, intermediate times in the range  $t_a < t < t_b$  are precisely determined by the times of the end segments:

$$t = t_a + (t_b - t_a) \frac{z - z_a}{z_b - z_a}$$
(A.24)

This gives a posterior based only on the likelihoods and the constraints from equations A.24 and A.1:

$$p_u(\mathbf{t}|\mathbf{y}, \mathbf{z}) \propto p(\mathbf{y}|\mathbf{t}(t_a, t_b, \mathbf{z}))p_H(t_a, t_b)$$
(A.25)

In OxCal such a model would be defined using the commands:

where **za** and **zb** are suitably defined.

In this case the prior is again neutral with respect to the difference between  $t_a$  and  $t_b$ .

#### A.3.3 Poisson model deposition (P\_Sequence)

Finally we come to the case of the Poisson mediated  $P\_Sequence$ . Here the total number of events is assumed to be  $k(z_b - z_a) - 1$  plus the start and end events (a and b). This is made up of both modelled events  $t_i$  with defined depth  $z_i$  and N other accumulation events (which do not have model parameters associated with them) that are assumed to result in the accumulation of the sediment. The difference in z between each accumulation event is 1/k and so between two modelled events occurring at times  $t_i$  and  $t_{i+1}$  there are  $n_i = k(z_{i+1} - z_i) - 1$  accumulation events. Strictly speaking  $N = \sum_{i=a}^{b} n_i$  and  $n_i$ 

should be integer, however in the OxCal implementation they are taken to be real numbers with a minimum of 0. The modelled events are a subset of the accumulation events. The accumulation events can occur at any time between  $t_a$  and  $t_b$  and thus the probability distribution function, as for the *Sequence* model, is given by equation A.21. The chance that any one will occur between time  $t_i$  and time  $t_{i+1}$  is given by the integral of the function  $f_u(t')$  from equation A.21:

$$\int_{t_i}^{t_{i+1}} f_u(t')dt' = \left(\frac{t_{i+1} - t_i}{t_b - t_a}\right)$$
(A.26)

and so the probability that exactly  $n_i = k(z_{i+1} - z_i) - 1$  of them occur in the same interval is given by:

$$p_u(z_i, z_{i+1}|t_i, t_{i+1}, t_a, t_b, k) \propto {}_N C_{n_i} \left(\frac{t_{i+1} - t_i}{t_b - t_a}\right)^{n_i} \left(1 - \frac{t_{i+1} - t_i}{t_b - t_a}\right)^{N - n_i}$$

Furthermore the probability of exactly  $n_i$  events occurring in each of the intervals  $(t_i \text{ to } t_{i+1})$  is:

$$p_u(\mathbf{z}|\mathbf{t},k) \propto N! \prod_{i=a}^{b-1} \frac{1}{n_i!} \left(\frac{t_{i+1}-t_i}{t_b-t_a}\right)^{k(z_{i+1}-z_i)-1}$$

and we use Bayes theorem to give:

$$p_u(\mathbf{t}|\mathbf{z},k) \propto p_u(\mathbf{z}|\mathbf{t},k)p_u(\mathbf{t})$$

where the informed prior  $p_u(\mathbf{t})$  is from equation A.22 (still valid for the modelled events), we find that the overall informed prior:

$$p_u(\mathbf{t}|\mathbf{z},k) \propto \frac{\prod_{a=1}^{b-1} (t_{i+1} - t_i)^{k(z_{i+1} - z_i) - 1}}{(t_b - t_a)^{k(z_b - z_a) - 1}}$$
(A.27)

Thus for a single segment of this form the overall posterior would be:

$$p_u(\mathbf{t}|\mathbf{y}, \mathbf{z}, k) \propto p(\mathbf{y}|\mathbf{t}) p_u(\mathbf{t}|\mathbf{z}, k) p_H(\mathbf{t})$$
 (A.28)

In OxCal such a model would be defined using the commands:

```
P_Sequence(k)
{
Boundary("a"){ z= za; };
```

```
Boundary("b"){ z=zb; };
};
```

where k, za and zb are suitably defined.

Once again this prior is neutral to the overall length of the segment  $t_b - t_a$  because of the number of possible combinations of  $k(z_b - z_a) + 1$  events (which includes the two boundaries) is proportional to  $(t_b - t_a)^{k(z_b - z_a) - 1}$ .

In the case of the  $U\_Sequence$  and the  $P\_Sequence$  the depth dependency of the model is independent of the number of modelled events (assuming this is less than the total number of events  $k(z_b-z_a)-1$  postulated in the sequence; if it is greater than the formulation of the model will break down). However, this is not the case in the Sequence model where the more events are introduced into the model, the more rigidly uniform the deposition will be. Another way of looking at the  $P\_Sequence$  is that it is the same as a Sequence model where one event is defined for each unit of deposition (ie each unit of depth 1/k). And again the  $U\_Sequence$  corresponds to the limit of an infinite event density.

## A.3.4 Multiple segments

So far we have only considered one segment of a deposition sequence. In many cases it may make sense to break a sedimentary sequence into several segments. In such cases each segment is treated independently although frequently the end of one segment will be coincident with the start of the next. Where the boundaries between segments are made is down to the judgement of the sedimentologist since this needs to be based on an assessment of the sediments themselves. What they should look for is evidence that the mode of sedimentation has changed. Because this is a matter of judgement it may be necessary to try more than one model and see how sensitive the end results are to these boundaries.

Mathematically one property that we would like the models to have is that our prior for the overall length of the depositional sequence should be independent of the number of intermediate boundaries. If the first boundary is at time  $t_a$  and the final boundary at  $t_m$ , each of the internal boundaries has a uniform prior which is defined as:

$$p(t) = \begin{cases} \frac{1}{t_m - t_a} & t_a < t < t_m \\ 0 & \text{otherwise} \end{cases}$$

and for n internal boundaries between the two outer boundaries  $t_a$  and  $t_m$ ,

the overall prior is proportional to:

$$p(t_a, t_m | n) = \frac{1}{(t_m - t_a)^n}$$
(A.29)

which, since the total number of possible combinations of n + 2 boundary dates is proportional to  $(t_m - t_a)^n$  gives a prior for the overall span which is independent of the number of internal boundary divisions defined for the model. In OxCal this factor is applied as long as the 'Uniform span prior' option is set.

The final factor in the prior comes from the fact that in practice the overall sedimentary sequence is sometimes constrained within outer limits. In the case that there is a lower limit  $llim_a$  for  $t_a$  and an upper limit  $ulim_m$  for  $t_m$  the number of possible combinations of solutions is proportional to:

$$g(t_a, t_m, llim_a, ullim_m) = (ulim_m - llim_a) - (t_m - t_a)$$
(A.30)

and so the reciprocal of this can be added as a prior factor (these latter two factors were suggested in Nicholls and Jones (2001) and Jones and Nicholls (2002) and are incorporated in OxCal prior to version 4 as described in Bronk Ramsey (2001)). If there is also an upper limit  $ulim_a$  for  $t_a$  and a lower limit  $llim_m$ for  $t_m$  the number of possible combinations becomes:

$$g(t_a, t_m, llim_a, ullim_m, ullim_a, ullim_m)$$

$$= \min((ulim_m - llim_a) - (t_m - t_a),$$

$$(t_m - t_a) - (llim_m - ulim_a),$$

$$ulim_a - llim_a,$$

$$ulim_m - llim_m)$$
(A.31)

and so the reciprocal of this quantity:

$$p(t_a, t_m | llim_a, llim_m, ullim_a, ullim_m) = \frac{1}{g(t_a, t_m, llim_a, llim_m, ullim_a, ullim_m)}$$
(A.32)

that is added as a prior factor in OxCal v4. When  $ulim_a = ulim_m$  and  $llim_a = llim_m$  the factors from equations A.30 and A.31 are identical.

#### A.4 Other underlying deposition scenarios

So far we have considered deposition processes which are on average uniform. There are some situations in which this is clearly inappropriate. In particular where we have sedimentation in depressions (for example filling of ditch features in an archaeological context), peat deposition (see example 1 in Christen et al. (1995)), accumulation restarting after a hiatus or sedimentation rate varying with climatic instability (as in Blockley et al. (2004)) we would expect some long-term trends. Likewise if we look at age depth models for ice cores, these would need to take into account the compression of the ice at lower levels.

The mathematical formulation for two further sets of deposition models will be considered here: linear and exponential rises in accumulation rate (these are easily extended to cover falls in accumulation rate).

#### A.4.1 Linear rise in accumulation rate (start point known)

If we postulate that the deposition rate starts from zero at time  $t_a$  and depth  $z_a$  and increases linearly until time  $t_b$  and depth  $z_b$ , we can replace the prior given in equation A.21 with the function:

$$f_l(t') = \begin{cases} 2\left(\frac{t'-t_a}{(t_b-t_a)^2}\right) & t_a < t' < t_b \\ 0 & \text{otherwise} \end{cases}$$
(A.33)

and thus we find that the prior for a simple sequence based on this model is the constraint prior  $p_H(\mathbf{t})$  multiplied by:

$$p_l(\mathbf{t}) \propto \prod_{i=a+1}^{b-1} \left( \frac{t_i - t_a}{(t_b - t_a)^2} \right) \tag{A.34}$$

Such a model would be defined in OxCal using the code:

```
Sequence()
{
  Zero_Boundary("a");
  ...
  Boundary("b");
};
```

For a  $U_-Sequence$  we define the accumulation rate within the time  $t_a < t < t_b$  to be:

$$\frac{dz}{dt} \propto f_l(t) \propto (t - t_a)$$

which, if we once more choose  $t_a$  and  $t_b$  to be our independent variables, gives an exact equation for t(z) in the range  $z_a < z < z_b$ :

$$t = t_a + (t_b - t_a) \sqrt{\frac{z - z_a}{z_b - z_a}}$$
(A.35)

This model would be defined in OxCal using the code:

```
U_Sequence()
{
   Zero_Boundary("a"){ z= za; };
   ...
   Boundary("b"){ z=zb; };
};
```

where **za** and **zb** are suitably defined.

For a *P\_Sequence* based on this deposition scenario we need to to replace equation A.26 with the integral of  $f_l(t')$  from equation A.33:

$$\int_{t_i}^{t_{i+1}} f_l(t')dt' = \left(\frac{t_{i+1}^2 - t_i^2 - 2t_a t_{i+1} + 2t_a t_i}{(t_b - t_a)^2}\right)$$
$$= \left(\frac{(t_{i+1} - t_a)^2 - (t_i - t_a)^2}{(t_b - t_a)^2}\right)$$
(A.36)

We can then follow through the same arguments that led to equation A.27 to find that the overall prior associated with the deposition model is the constraint prior  $p_H(\mathbf{t})$  multiplied by:

$$p_{l}(\mathbf{t}|\mathbf{z},k) \propto \frac{\prod_{i=a}^{b-1} \left( (t_{i+1} - t_{a})^{2} - (t_{i} - t_{a})^{2} \right)^{k(z_{i+1} - z_{i}) - 1} \prod_{i=a+1}^{b-1} (t_{i} - t_{a})}{(t_{b} - t_{a})^{2(k(z_{b} - z_{a}) - 1)}}$$
(A.37)

Such a model would be defined in OxCal with the code:

```
P_Sequence(k)
{
```

```
Zero_Boundary("a"){ z= za; };
...
Boundary("b"){ z=zb; };
};
```

where k, za and zb are suitably defined.

#### A.4.2 Linear rise in accumulation rate (start point not known)

If  $z_a$  (the depth at which the accumulation rate started from zero) is unknown we can allocate a uniform prior for  $t_a$  and assume that all of the deposition events occur in the depth range,  $z_{a+1}$  to  $z_b$  and in the time interval  $t_{a+1}$  to  $t_b$ . The underlying prior probability for an accumulation event then becomes:

$$f_{l^*}(t') = \begin{cases} 2\left(\frac{t'-t_a}{(t_b-t_a)^2 - (t_{a+1}-t_a)^2}\right) & t_{a+1} < t' < t_b \\ 0 & \text{otherwise} \end{cases}$$
(A.38)

For a *U\_Sequence* we define the accumulation rate within the time  $t_{a+1} < t < t_b$  to be:

$$\frac{dz}{dt} \propto f_{l^*}(t) \propto (t - t_a)$$

However in this case  $z_a$  is unknown. We therefore have three independent variables which we will choose to be  $t_a$  (the time at which deposition starts)  $t_{a+1}$  (the first time for which we have depth information) and  $t_b$  (the end of the sequence). Solving the differential equation subject to these conditions we obtain an exact equation for t(z) in the range  $z_{a+1} < z < z_b$ :

$$t = t_a + (t_b - t_a) \sqrt{1 - \left(\frac{z - z_b}{z_{a+1} - z_b}\right) \left(1 - \left(\frac{t_a - t_{a+1}}{t_a - t_b}\right)^2\right)}$$
(A.39)

This model would be defined in OxCal using the code:

```
U_Sequence()
{
  Zero_Boundary("a");
  ...
  Boundary("b"){ z=zb; };
};
```

where zb is suitably defined.

For a *P\_Sequence* we need to substitute for equation A.26 the integral of the function  $f_{l^*}(t')$ :

$$\int_{t_i}^{t_{i+1}} f_{l^*}(t')dt' = \frac{(t_{i+1} - t_a)^2 - (t_i - t_a)^2}{(t_b - t_a)^2 - (t_{a+1} - t_a)^2}$$
(A.40)

and using this the overall prior is the constraint prior  $p_H(\mathbf{t})$  multiplied by:

$$p_{l^*}(\mathbf{t} \mid z_{a+1}, \cdots, z_b, k) \\ \propto \frac{\prod_{i=a+1}^{b-1} \left( \left( (t_{i+1} - t_a)^2 - (t_i - t_a)^2 \right)^{k(z_{i+1} - z_i) - 1} (t_i - t_a) \right)}{((t_b - t_a)^2 - (t_{a+1} - t_a)^2)^{k(z_b - z_{a+1}) - 1}}$$
(A.41)

Such a model would be defined in OxCal with the code:

### A.4.3 Exponential rise in accumulation rate

If instead the deposition rate is expected to increase exponentially we can formulate the model in the following way. We define  $t_b$  as the endpoint of the distribution and  $t_a$  to be one time constant earlier. In this case, the constraints are different from those given in equation A.1 in that the only constraint on  $t_a$ is that  $t_a < t_b$ . The prior for a single deposition event, which can be substituted for the function in equation A.21, is then:

$$f_e(t') = \begin{cases} \left(\frac{e^{-(t'-t_b)/(t_a-t_b)}}{t_b-t_a}\right) & -\infty < t' < t_b \\ 0 & \text{otherwise} \end{cases}$$
(A.42)

Using this, the overall prior for a single-segment sequence, including the constraints is:

$$p_e(\mathbf{t}) \propto p_H(t_a, t_b) p_H(t_{a+1}, \cdots, t_b) \prod_{i=a+1}^{b-1} \left( \frac{\exp\left(-\frac{t_i - t_b}{t_a - t_b}\right)}{t_b - t_a} \right)$$
 (A.43)

Such a model would be defined in OxCal using the code:

```
Sequence()
{
  Tau_Boundary("a");
  ...
  Boundary("b");
};
```

For a  $U_Sequence$  we define the accumulation rate within the time range  $-\infty < t < t_b$  to be:

$$\frac{dz}{dt} \propto f_e(t) \propto e^{-(t-t_b)/(t_a-t_b)}$$

We again have three independent variables which we will choose to be  $t_a$  (one time constant before  $t_b$ )  $t_{a+1}$  (the first time for which we have depth information) and  $t_b$  (the end of the sequence). Solving the differential equation subject to these conditions we obtain an exact equation for t(z) in the range  $z_{a+1} < z < z_b$ :

$$t = t_b - (t_a - t_b) \ln \left( 1 - \left( \frac{z - z_b}{z_{a+1} - z_b} \right) \left( 1 - \exp \left( -\frac{t_{a+1} - t_b}{t_a - t_b} \right) \right) \right)$$
(A.44)

This model would be defined in OxCal using the code:

```
U_Sequence()
{
  Tau_Boundary("a");
  ...
  Boundary("b"){ z=zb; };
};
```

where zb is suitably defined.

For a *P\_Sequence* based on this exponentially rising deposition model we consider only those deposition events which occur between the depths  $z_{a+1}$  and  $z_b$ . For those the normalised probability is:

$$f_{e^*}(t') = \begin{cases} \frac{\left(\exp\left(-\frac{t'-t_b}{t_a-t_b}\right)\right)}{\left(1-\exp\left(-\frac{t_{a+1}-t_b}{t_a-t_b}\right)\right)(t_b-t_a)} & t_{a+1} < t' < t_b \\ 0 & \text{otherwise} \end{cases}$$
(A.45)

We must once again substitute for equation A.26 the integral of the function  $f_{e^*}(t')$ :

$$\int_{t_i}^{t_{i+1}} f_{e^*}(t')dt' = \frac{\exp\left(-\frac{t_{i+1}-t_b}{t_a-t_b}\right) - \exp\left(-\frac{t_i-t_b}{t_a-t_b}\right)}{1 - \exp\left(-\frac{t_{a+1}-t_b}{t_a-t_b}\right)}$$
(A.46)

We can then follow through the same arguments that led to equation A.27 to find that the overall prior associated with the deposition model including the constraints is proportional to:

$$p_{e} (\mathbf{t}|z_{a+1}, \cdots, z_{b}, k) \propto$$

$$p_{H}(t_{a}, t_{b})p_{H}(t_{a+1}, \cdots, t_{b}) \times$$

$$\frac{\prod_{i=a+1}^{b-1} \left( \left( \exp\left(-\frac{t_{i+1}-t_{b}}{t_{a}-t_{b}}\right) - \exp\left(-\frac{t_{i}-t_{b}}{t_{a}-t_{b}}\right) \right)^{k(z_{i+1}-z_{i})-1} \left( \frac{\exp\left(-\frac{t_{i}-t_{b}}{t_{a}-t_{b}}\right)}{t_{b}-t_{a}} \right) \right)}{\left( 1 - \exp\left(-\frac{t_{a+1}-t_{b}}{t_{a}-t_{b}}\right) \right)^{k(z_{b}-z_{a+1})-1}}$$
(A.47)

Such a model would be defined in OxCal with the code:

```
P_Sequence(k)
{
   Tau_Boundary("a");
   ...
   Boundary("b"){ z=zb; };
};
```

## A.5 Summary of mathematical methods

We are able to derive a mathematical *prior* probability for all of the models described in table 1. In many cases this is actually only a factor in this probability (in other words it is unnormalised) but fortunately for MCMC analysis this is all that is required.

Table 1 refers to the equations specifying the prior for each of the main models (together with factors from equations A.29 and A.32 if required). When taken together with the *likelihood* distributions (see section 3.1) and the constraints (as given in equation A.1) these define the probability function for the model as a whole.

The mathematical formulation for Sequence,  $U\_Sequence$  and  $P\_Sequence$  models can also be derived for linear and exponential increase or decrease as

shown here. In all cases they can be derived so that the prior for the overall scale of the sequence is neutral. These models are all implemented in OxCal v4.

# **B** Binomial treatment of Ice-Core uncertainties

For each uncertain layer which might correspond to either zero or one year we can treat this as a Bernoulli trial which is either false or true. We assume the probability that the layer is real is p and the probability that it is not is q = 1 - p. For a whole segment of core with N uncertain layers it then follows that the probability that there are exactly n real extra layers in the segment is given by:

$$P_p(n|N) = \frac{N!}{n!(N-n)!} p^n (1-p)^{N-n}$$

The mean of this distribution is  $\mu = Np$  as you would expect. It also turns out that if N is high enough this approximates to a normal or Gaussian distribution with a variance of:

$$\sigma^2 = Np(1-p)$$

that is we get:

$$P_p(n|N) \approx \frac{1}{\sqrt{2\pi N p(1-p)}} \exp\left(-\frac{(n-Np)^2}{2N p(1-p)}\right)$$

In practice if we assume that p (and therefore q) are 0.5 the situation further simplifies and for N uncertain layers we get the following results:

- The mean expected number of layers is N/2
- The probability distribution is approximately normal with a standard uncertainty of  $\sqrt{N}/2$
- The 95% confidence range is  $\pm \sqrt{N}$

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