

The Holocene

<http://hol.sagepub.com>

Relationships between calibrated ages and depth in stratigraphical sequences: an estimation procedure by mixed-effect regression

Einar Heegaard, H. J.B. Birks and Richard J. Telford

The Holocene 2005; 15; 612

DOI: 10.1191/0959683605hl836rr

The online version of this article can be found at:
<http://hol.sagepub.com/cgi/content/abstract/15/4/612>

Published by:

 SAGE Publications

<http://www.sagepublications.com>

Additional services and information for *The Holocene* can be found at:

Email Alerts: <http://hol.sagepub.com/cgi/alerts>

Subscriptions: <http://hol.sagepub.com/subscriptions>

Reprints: <http://www.sagepub.com/journalsReprints.nav>

Permissions: <http://www.sagepub.com/journalsPermissions.nav>

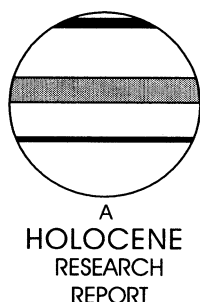
Citations (this article cites 19 articles hosted on the SAGE Journals Online and HighWire Press platforms):
<http://hol.sagepub.com/cgi/content/refs/15/4/612>

Relationships between calibrated ages and depth in stratigraphical sequences: an estimation procedure by mixed-effect regression

Einar Heegaard,^{1,2*} H.J.B. Birks^{1,2,3} and Richard J. Telford¹

¹Bjerknes Centre for Climate Research, University of Bergen, Allégaten 55, 5007 Bergen, Norway; ²Biological Institute, University of Bergen, Allegaten 41, 5007 Bergen, Norway; ³Environmental Change Research Centre, University College London, 26 Bedford Way, London WC1H 0AP, UK)

Received 1 October 2003; revised manuscript accepted 8 June 2004



Abstract: We present a procedure for estimating age–depth relationships in stratigraphical sequences by means of a generalized mixed-effect regression using an ancillary function for the partitioning of the fixed effect and the random effect corresponding to the degree of representativity of the individual calibrated dates for a particular section of the sedimentary sequence. The procedure uses mid-point estimates of the calibrated ages in combination with the central distributional range as the basis for estimating the fixed relationship between age and depth. Further, it combines the variability of the calibrated age at individual layers (within-object variance) with estimation of the variability of the calibrated age distribution as a whole between the layers standardized by the fixed effect (between-object variance). These components of random variability can be considered independent, and hence the uncertainty of the estimated fixed relationship between age and depth can be estimated by combining the two random variables. The procedure follows the logic of mixed-effects models, but with prior information about the expected variance within each dated object.

Key words: Sediment sequences, age–depth relationships, GAM, mixed effects, calibrated ages.

Introduction

In palaeoecology and palaeoclimatology keys to any inference about historical records are the times of particular events the time between events, the duration of such events and the rates of changes. These temporal issues have led to a great interest in the fields of ¹⁴C dating (Boaretto *et al.*, 2002), ²¹⁰Pb dating (Appleby, 2001), varved records (Brauer *et al.*, 2001), and other dating methods. These procedures are expensive and time-consuming, and frequently materials from sediment cores are poor in quality or quantity for particular procedures. Nevertheless, as we are interested in the entire historical sequence, we wish to extract information from dated points that is applicable to the rest of the core, i.e., by finding the relationship between the depths of the sediment sequence and their ages. To estimate such age–depth relationships, several statistical techniques have been proposed, e.g., various regression techniques (Maher, 1972; Bennett, 1994; Bennett and Fuller, 2002) and

fuzzy-regression (Boreux *et al.*, 1997). The key difficulties that these procedures consider are how to find the expected age at a particular depth and, more importantly, what is the uncertainty of the particular estimate. The importance of the latter is obvious, as a statement about the age of an event has very different meanings if we say the age will most likely lie within a 50-year interval or within a 200-year interval.

Most procedures estimate the error by an assumed distribution of the central points of a calibrated depth, or by a bootstrap procedure of observations from the calibrated distributions (see Bennett, 1994; Telford *et al.*, 2004a). Alternatively, a Bayesian procedure estimates the probability density distribution, i.e., posterior probability, of the calibrated age using the calibrated distributions (see Buck *et al.*, 1996). We fully recognize the potential advantages of the Bayesian approach in finding reliable estimates of the probability density function for ages at dated depths. Nevertheless, we formalize here a procedure that highlights some additional aspects of estimating age–depth relationships, namely the uncertainty related to how representative the dated object is in relation to

*Author for correspondence (e-mail: einar.heegaard@bio.uib.no)

the sampled layer, and not just the error estimates of the individual dated object (objects here are organic material submitted for dating). The procedure has not been fully described before, although it has been applied in several published studies (e.g., Rosén *et al.*, 2001; Seppä and Birks, 2001, 2002; Bigler *et al.*, 2002; Seppä *et al.*, 2002; Heiri *et al.*, 2003a, b), and functions for the statistical software S-plus and R are available (Heegaard, 2003). The procedure can be characterized as a mixed-effect model as it includes both a fixed effect, namely the ‘influence’ of depth on age, and two random effects, first related to the dating of the objects (within-object variance), and secondly related to how representative the dated objects are in relation to the section of the sequence from where they were sampled (between-object variance).

Calibrated age to depth relationship as a mixed-effect model

The data for modelling

The dating of a sediment sequence by radiocarbon dating involves submitting organic material (objects) from selected layers to a dating laboratory. From the laboratory we receive the estimated radiocarbon age with an uncertainty for each of the objects in radiocarbon years BP. As radiocarbon years do not correspond to calendar years, we need to transform or calibrate these observations into calibrated ages. For this, the software Calib (Stuiver and Reimer, 1993), Oxcal (Ramsey, 2001), or Bcal (Buck *et al.*, 1996) are frequently used. Although radiocarbon years are normally distributed, the calibrated years are not normally distributed owing to a non-linear transformation function. For simplicity here, we assume various procedures for finding a central distributional range and the central point of these distributions (see Telford *et al.*, 2004a). Telford *et al.* found that a central point either as the median or the weighted mean of the central 68% range gives reasonable estimates in comparison with the widely used intercept method of calibration. We can obtain a central point and an uncertainty (variance) for each dated sample, i.e., within-object variance. However, an important question in this context is does the object dated reflect the layer from which it is picked? This is important because of the aim, namely, making a statement about the layers throughout the sequence. Obviously if the object is either contaminated or transported within the sequence (up or down), or some sedimentary disturbance has occurred (e.g., missing layers, erosion, etc.), there will be a misrepresentation. In addition, the object selected is frequently only a minor part of all the possible objects that could be estimated at a particular layer. By selecting a different object from the same layer a different radiocarbon estimate may be obtained. This type of variability is in addition to the variability of the dating process of the submitted object, and must be included as a part of the overall uncertainty of the final estimated relationship. Thus, there are at least two general sources of error involved: (1) the error of the particular object dated, i.e., within-object error, and (2) the potential error of the object to layer relationship, i.e., between-object error, which is influenced by processes within the sequence (contamination, object transport, turbidites, hiatuses, etc.) and the random difference between objects of the same population.

Mixed modelling

A mixed-effect model is defined as a model that includes both a fixed variable, i.e., a particular variable that determines the expected response, and a random variable, which describes the variability of some group of observations in addition to the

individual observations themselves (see Pinheiro and Bates, 2000). The fixed variable, which is the predictor variable in a classic linear model, tells us how the expected response will differ as the conditions described by the predictor variable change. The degree of change is identified as the fixed effect. A random variable is a variable that describes a property of the distribution for the underlying population from which the different observations are gathered.

To formalize the calibrated age–depth relationship including a fixed depth and the two sources of variance (random effects), we can view the relationship as a fixed-effect function in combination with a between-object random factor and a within-object random factor:

$$\text{Cage}_{ji} = f(\text{depth}_j) + b_{0j} + \varepsilon_{ji} \quad (1)$$

where Cage_{ji} is the i th possible calibrated age at the j th dated object, $f(\text{depth}_j)$ is a fixed effect, and b_{0j} is the random effect for dated objects being selected from a population of objects at that layer and a population of depths to be selected (between-object), whereas ε_{ji} represents the random effect related to the calibrated age estimate of the j th submitted object (within-object). It is important here to recognize that b_{0j} in general follows a normal distribution with zero mean and sigma squared variance ($N(0, \sigma_b^2)$). Further, we can assume that b_{0j} and ε_{ji} are independent, and hence the variance related to the response is additive (see Pinheiro and Bates, 2000):

$$\text{var}(\text{Cage}_{ji}) = \sigma_b^2 + \sigma_\varepsilon^2$$

From the calibrated age distribution representing the individual object we know the individual variability (σ_ε^2). Thus we only need to estimate the fixed relationship of the calibrated age–depth relationship and the random effect inherent in the different layers dated. However, as we only have one object dated at each layer, how can we estimate the uncertainty of the layers dated? To solve this we utilize the additivity of the terms in Equation (1). The expected calibrated year for the objects dated can be described as:

$$E(\text{Cage}_j) = f(\text{depth}_j) + b_{0j} \quad (2)$$

This simplification of Equation (1) is the observed central point of the j th layer as a function of some fixed function of depth and some random variability between objects (σ_b^2). Equation (2) can be solved by various regression procedures, including polynomial regression and various smoothers, with the central points of each object as the response variable, i.e., $E(\text{Cage}_j) = \mu_j = j$ th central point. As b_{0j} is assumed to be normal, the variance σ_b^2 is given by the mean sum of squares for Equation (2). Note that the subscript reflects the j th layer, which suggests that this part of the system amounts to Σ_j number of observations, which is logical as all ‘observations’ for each object have the same depth. Having estimated the fixed function ($f(\text{depth}_j)$) and the corresponding random effect (b_{0j}), we can describe the relationship between the calibrated age and depth by substituting Equation (2) into Equation (1):

$$E[E(\text{Cage}_j)] = E(\text{Cage}_{ji}) = f(\text{depth}_j) \quad (3)$$

with the variance:

$$\text{var}(\text{Cage}_{ji}) = \sigma_b^2 + \sigma_\varepsilon^2$$

From these values we can then estimate the confidence intervals following standard statistical procedures (Myers *et al.*, 2002)

$$E(\text{Cage}_{ji}) \pm Z_{\alpha/2} \sqrt{\text{var}(\text{Cage}_{ji})} \\ \times \sqrt{[\text{depth}_{ji}^T (\text{Depth}^T \text{Depth})^{-1} \text{depth}_{ji}]} \quad (4)$$

where $E(\text{Cage}_{ji})$ is the predicted age at the j th dated object and i th possible calibrated age, $Z_{\alpha/2}$ is the critical value of a standard Normal distribution corresponding to significance level α , $\text{var}(\text{Cage}_{ji})$ is the variance of the predicted response at j th dated object, and depth_{ji} is the depth at the j th dated object, and Depth is the model matrix including an intercept column and depth as a column. The expression $[\text{depth}_{ji}^T (\text{Depth}^T \text{Depth})^{-1} \text{depth}_{ji}]$ describes the position of the j th dated object in relation to the distribution of all dated objects.

An example: age–depth relationship at Storsandsvatnet, western Norway

As seen above, the estimation of the calibrated age–depth relationship is based on several steps.

- (1) Estimate a central point of the calibrated age and the within-object variance (σ_e^2).
- (2) By regression, find the relationship between the central points and sediment depth. This gives the expected calibrated ages at the various depths.
- (3) Estimate the between-object variance (σ_b^2) from the regression (step 2).
- (4) Estimate the variance of the expected calibrated ages by summing the variances from stages 1 and 2.
- (5) Calculate the 95% confidence interval for each age estimate at each depth.

The example follows the procedure provided by the *Cagedepth.fun* function (Heegaard, 2003) for Windows-versions of the statistical software R (<http://cran.r-project.org/>; last accessed 22 February 2005). Organic material from 11 layers throughout the sequence spanning the entire Holocene was dated from a core in Storsandsvatnet, western Norway (63°27'N, 8°27'E) (H.J.B. Birks and S.M. Peglar, unpublished dates).

Step 1. From the radiocarbon laboratory we received 11 radiocarbon dates, which were individually calibrated using Oxcal (Ramsey, 2001). From the calibrated distribution we found the central 68% percentage range, and the central point by mid-point of the ranges. This procedure gives us a table of the depth and the younger and older calibrated age (Table 1), which is the basis for our estimations of the fixed effect, and the two random components. For the variance of the individual object (σ_e^2) we need the assumption that the central 68% percentage integral of a calibrated distribution reflects the central point \pm standard deviation (sd). Then the variance of the individual object is $\sigma_e^2 = \text{sd}^2$. Owing to the independence of the central point and variance, we then extract the central points to be regressed against depth.

Step 2. To solve Equation (2) of the previous section by regression of the central points against depth we assume a normal distribution (although in very rare cases this is not sufficient). In estimating $f(\text{depth}_{ji})$ we can use any regression procedure, including polynomial terms, and a variety of smoothers such as natural splines, cubic smooth splines, etc. In addition, there are many criteria for selecting the ‘best-fit’ relationship, such as F-statistics, AIC, BIC, cross-validation, etc. (Hastie *et al.*, 2001). Note that the choices made for polynomial terms or smoothers, and the selection criterion can give different results.

In *Cagedepth.fun* we use a cubic smooth spline function, including a knot at each dated layer as the start for the shrinkage process (Wood, 2000, 2001; Hastie *et al.*, 2001). As a criterion for the model selection, i.e., ‘best-fit’, we used the Generalized Cross-Validation provided by Wood (2001) in the *mgcv* library of R (<http://cran.r-project.org/>; last accessed 22 February 2005). Further, as a check for the assumption of normality between-object variance, we have included diagnostic plots for two separate models; (1) constant variance (Normal distribution), and (2) variance as a function of the expected mean (Poisson-like distribution). To be able to generate these regressions we use a Generalized Additive Model (GAM; Hastie and Tibshirani, 1990; Wood, 2001) with a quasi-likelihood distribution. This procedure allows an identity link between the linear predictor and the expected response to be combined with different variance functions (see Firth, 1991). The diagnostic plots are used for comparison between the two options, and we would only use option 2 if there is clear evidence for this being a significant improvement (very rarely observed). If there are no differences between the two options, we select option 1 as is the case for the example (Figure 1). The expected calibrated ages for both models are given in the numerical output of *Cagedepth.fun* (Table 2).

Step 3. Having solved Equation (2) and found the ‘best-fit’ relationship between the central calibrated ages and depth, we use these results to find the between-object variance (σ_b^2). For generalized models the variance can be expressed as: $\text{var}(y_i) = \phi V(\mu)$, where ϕ is a scale parameter (σ^2 for Normal distribution), and $V(\mu)$ is a description of the mean to variance relationship (McCullagh and Nelder, 1989; Firth, 1991). For the two options the variances are: (1) $\sigma_b^2 = \sigma^2 V(\mu)$, where $V(\mu) = 1$ (constant) and $\sigma^2 = \text{MSres}$, (2) $\sigma_b^2 = \phi V(\mu)$, where $V(\mu) = \mu$ (expected mean) and $\phi =$ standardized squared Pearson residuals (Venables and Ripley, 2002). The variances for both options are given in the numerical output of *Cagedepth.fun* (Table 2).

Step 4. Having obtained an estimate of both random components, b_{0j} and ε_{ji} , we can determine the variance of the expected calibrated age by summing these independent variables:

$$\text{var}(\text{Cage}_{ji}) = \sigma_b^2 + \sigma_e^2$$

This procedure models the variability of the individual point in the calibrated age distribution as a function of the variance between objects and of the variance within the object (Table 2).

Table 1 The input information to the *Cagedepth.fun* function

depthup	depthdo	cageup	cagedo
69.5	70.5	– 56	– 46
119.5	120	3465	3565
156.6	157	5775	5925
204.5	205	6760	6900
244.5	245	8410	8625
274.5	275	9005	9085
296.5	297	7880	8010
314.5	315	10235	10400
334.5	335	10605	11060
349.5	350	11255	11555
389.5	390.5	13450	13820

Depthup = upper depth of sampled layer (cm), depthdo = lower depth of sampled layer (cm), cageup = younger border of 68% central calibrated age distribution (calibrated years BP), cagedo = older border of 68% central calibrated age distribution (calibrated years BP).

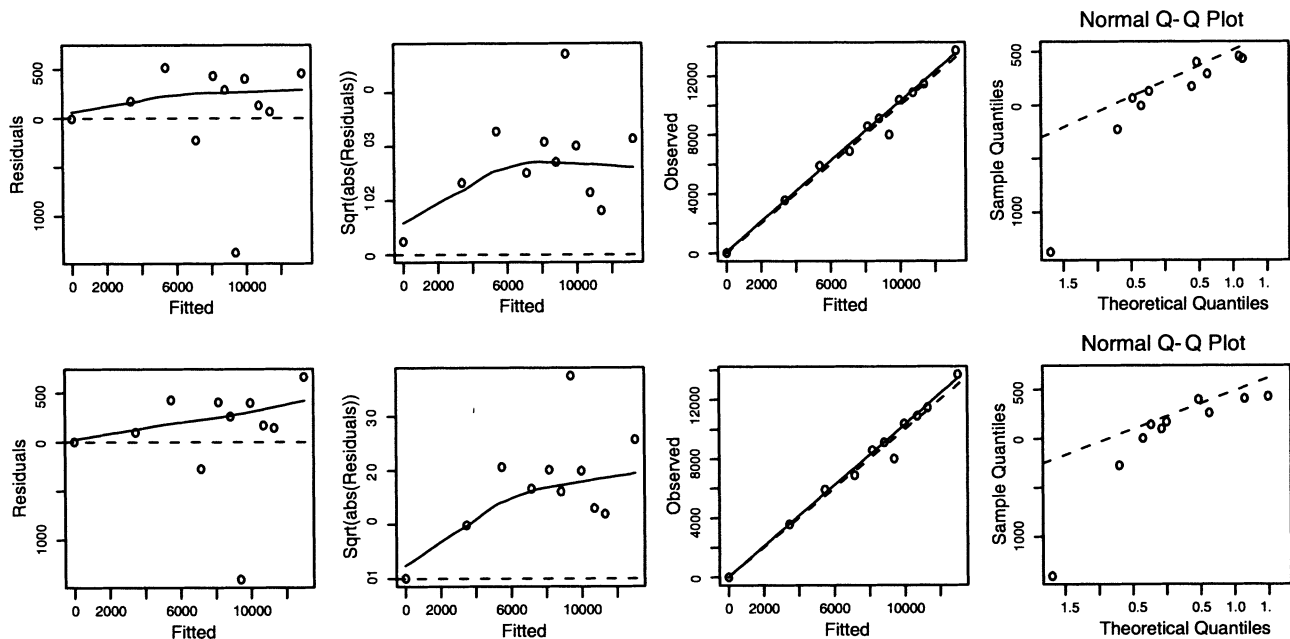


Figure 1 The diagnostic plots for the cubic smooth spline regression including the constant variance (row 1) and μ variance (row 2). The diagnostic plots include column-wise; residuals versus fitted values (no trend), square root of absolute residuals versus fitted (no trend should appear), observed versus fitted (observations along the diagonal line), and a qq-normplot (observations along the diagonal line). Here we see that there are no differences between the two options and hence we select the simpler constant variance

Step 5. Combining all the information gathered so far produces an estimate of calibrated age–depth relationship with a 95% confidence interval (Figure 2 and Table 2) following Equation (4).

From the results of Storsandvatnet (Table 2, Figures 2 and 3) we see that there are no big differences between the two variance-function options. Hence, we select the simpler model based on constant variance. Note that by assuming a μ variance function (option 2), the uncertainty decreases more strongly towards today, but a higher variance is assigned to the older dates. The function Cagedepth.fun only gives numerical output for the dated layers. To be able to expand this information to other layers of the core we have provided an additional function Cagenew.fun. This function uses numerical information from the Cagedepth.fun function to calculate age estimates for all the sediment depths required. Both functions can be found within the downloadable file CagedepthR.txt at the HOLIVAR homepage (<http://geog.ucl.ac.uk/ccrc/holivar/utrecht.htm>; last accessed 22 February 2005), or at EECRG home page (<http://www.uib.no/bot/qeprg/Age-depth.htm>; last accessed 22 February 2005).

Discussion

The procedure presented here differs from previous age–depth estimation procedures (Bennett, 1994; Buck *et al.*, 1996; Boreux *et al.*, 1997; Bennett and Fuller, 2002) by an explicit attempt to estimate the variability between dated objects at the different layers of the sequence. Hence, we try to derive a measure of how representative each dated object is in relation to the population from which it is sampled. This variability comes in addition to the uncertainty of the radiocarbon dating of the individual object. Thus, obviously we need an estimate of both these types of variance to be able to derive a reasonable error estimate for the final calibrated age–depth relationship. The impact of the procedure is seen by the inference of the

system. Without taking account of the between-object variability, we treat the calibrated-age distribution as fixed for that particular layer. Next we infer a relationship between calibrated ages and objects rather than a calibrated age to depth relationship. Our procedure relaxes the assumption required by previous procedures (Maher, 1972; Bennett, 1994; Boreux *et al.*, 1997; Bennett and Fuller, 2002), namely that the objects dated are themselves accurate representations for particular layers. By relaxing this assumption and explicitly estimating the variability between objects we expand the confidence interval, as the variance now comprises two components. The inclusion of both types of errors (within-object and between-object) allows the uncertainty in the system of age–depth relationships through the core, being expressed not only as a function of errors related to the radiocarbon dating process, but also as errors related to layers and dated objects within layers, such as contamination, inaccurate depth measurement, etc. This makes the difference in interpretation from previous procedures, as we do not consider each dated object as fixed focusing on the relationship of the dated objects, but consider the population of possible dated objects to infer for the whole stratigraphical sequence. However, the procedures will numerically approximate each other when the central points can be replicated exactly by the fixed function used in Equation (2), as the between-object variability will then be negligible. Nevertheless, we find it reassuring that the different potential sources of variability are accounted for, and the inference is in the calibrated age–depth relationship.

However, the procedure as described here, and for which functions are provided (Heegaard, 2003) makes some assumptions. As the radiocarbon dates are normally distributed, and hence the mean and variance are independent, and as this is a property we need to include, we assume that the transfer function is linear within the standard deviation range of the radiocarbon dates. This procedure equals that of a 68% central range based on the central point, which is a reasonable estimate of the central points (Telford *et al.*, 2004a). This procedure will also ensure that the central point and the

Table 2 Parts of the numerical output from Cagedepth.fun

Variance	Depth	Cal.age	Est.age	Low.lim	Upp.lim	Tsd	Csd	Rsd
Constant	70.0	- 51.0	- 45.30	- 199.05	108.45	78.44	5.00	78.28
	119.8	3515.0	3339.44	2623.54	4055.34	365.25	50.00	361.82
	156.8	5850.0	5334.36	4517.82	6150.90	416.60	75.00	409.80
	204.8	6830.0	7057.09	6231.50	7882.68	421.22	70.00	415.36
	244.8	8517.5	8083.89	7317.04	8850.75	391.25	107.50	376.19
	274.8	9045.0	8753.74	8113.96	9393.52	326.42	40.00	323.96
	296.8	7945.0	9317.56	8673.61	9961.52	328.55	65.00	322.06
	314.8	10317.5	9914.85	9205.29	10624.42	362.02	82.50	352.50
	334.8	10832.5	10701.73	9775.01	11628.45	472.81	227.50	414.48
	349.8	11405.0	11339.43	10346.25	12332.61	506.72	150.00	484.01
390.0	13635.0	13178.80	11484.25	14873.36	864.57	185.00	844.54	
μ	70.0	- 51.0	- 51.00	- 61.46	- 40.54	5.34	5.00	1.87
	119.8	3515.0	3417.89	2887.19	3948.58	270.76	50.00	266.11
	156.8	5850.0	5424.08	4772.60	6075.57	332.39	75.00	323.82
	204.8	6830.0	7105.80	6366.42	7845.19	377.24	70.00	370.69
	244.8	8517.5	8113.73	7384.46	8843.00	372.08	107.50	356.21
	274.8	9045.0	8786.88	8154.88	9418.88	322.45	40.00	319.96
	296.8	7945.0	9346.96	8694.61	9999.32	332.83	65.00	326.43
	314.8	10317.5	9921.38	9186.90	10655.85	374.73	82.50	365.54
	334.8	10832.5	10665.02	9684.63	11645.41	500.20	227.50	445.47
	349.8	11405.0	11263.69	10174.33	12353.04	555.79	150.00	535.17
390.0	13635.0	12975.83	11080.44	14871.21	967.03	185.00	949.17	

Variance = the options of variance function used, Depth = depth of the sampled layer (cm), Cal.age = central point estimation of the calibrated age distribution (calibrated years BP), Est.age = estimated age for the individual layers sampled (calibrated years BP), Low.lim = younger 95% confidence interval (calibrated years BP), Upp.lim = older 95% confidence interval (calibrated years BP), Tsd = total standard deviation ($Tsd = \sqrt{Csd^2 + Rsd^2}$), Csd = calibrated age standard deviation (within object), Rsd = regression standard deviation (between object).

variance of the calibrated ages are independent. The assumption of linearity need not be constant, i.e., the slope of the transfer function may differ for neighbouring dated objects. Nevertheless, it is unclear at present if this assumption is really needed to obtain independence between the central point and the within-object variability, otherwise the complexity of the relationship increases dramatically. A second assumption is the distribution of the between-object variance. In very rare cases, diagnostic plots have shown that a normal distribution is an insufficient assumption for the estimation of the fixed effect and the between-object variability (Equation 2). Several reasons may account for this situation. For example, the lower parts of a core may have been exposed to disturbance or mixing for a longer period than the upper layers just because of their greater age. Such processes can increase the natural variability between dated objects, and we need to assume a relationship between the estimated mean and the variance. This relationship is solved by Generalized Models (McCullagh and Nelder, 1989; Hastie and Tibshirani, 1990) using a quasi-likelihood distribution that can combine various link-functions with different variance-functions (Firth, 1991). Of all the cases that we have encountered where the normal assumption has been insufficient, an identity link function combined with a μ variance function ($\text{var}(y) = \phi\mu$; see Firth, 1991) has provided an appropriate alternative.

A feature of the procedure presented here is the allowance for combining objects being dated by several different procedures, such as ^{14}C or ^{210}Pb dating, and also to include layers that we have specific *a priori* information about, such as top-layer = today, and tephra-layers with a very small within-object uncertainty. The only information needed is the central point of the object on a calibrated age scale and a measurement of the within-object uncertainty. Different inherent uncertainties of the different procedures will be accounted for by the weighted regression of Equation (2),

and we can also 'fix' estimation, i.e., making the estimation biased towards layers that are nearly precisely dated (top-layer, tephra-layers, etc.) by increasing the weights. In the Cagedepth.fun function such weights can be introduced, which by default are the inverse of the within-object variance. Further, a property of explicitly examining the between-object variability is that we can compare for each dated object the magnitude of the within-and between-error. From these comparisons we can gain information about the stratigraphical sequence and the individual object dated. If the between variability is large in comparison with the within variability we may have an outlier. An outlier is by definition

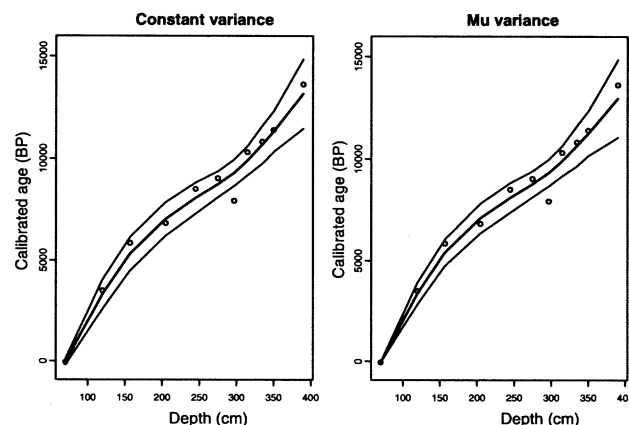


Figure 2 The expected age throughout the sequence (bold line) with 95% confidence intervals (thin lines) for the two models with different variance structure. In this example we select the constant variance. Note that the confidence interval of the μ variance model tends to be narrower towards the surface but wider with increasing age

an observation that is relatively far from the expected value in comparison to the general variance. Note that an object may be an outlier even though the within variance is minor. Such points should be carefully examined and the potential cause of the outlier sought. It may be the observation itself, but it may also be the specified relationship. In cases where there are missing sections in the sequence we can have an object at both sides that may both show a very low within variance. Owing to the missing section, these will be closer together in the depth axis than in reality, and the expected estimate may be somewhere between these observations, generating a high between-object variability. For such cases the best thing to do is to submit more objects for dating. In cases where we are certain of missing sections we can expand the fixed function of Equation (2) by a piecewise function, i.e., estimate a function with a discontinuity at the potential missing section (Hastie *et al.*, 2001). However, such procedures demand several dated objects present on both sides of the missing section. In relation to outliers, reversed observations have been discussed in several aspects. A reversed object is a date that, relative to the nearby objects, does not follow the law of superposition, i.e., an object found higher up in the core is older than the object below. This is seen by the seventh object in our example (Figure 2). In this example, there is a high probability that this object poorly represents the underlying sedimentology of the sequence. However, in many other cases it can be difficult to determine which of two points are ‘wrong’, i.e., the law of superposition is fulfilled if we take away either of these observations. Instead of deleting any of these observations, thereby creating a curve with a narrower confidence interval, we favour including both observations and rather state that within this section there is a large uncertainty in relation to the expected calibrated ages. However, as mentioned above the best thing to do is to obtain more information by submitting more samples for dating.

Conclusions

We see that the confidence intervals provided by this procedure are wider than previous estimation procedures, but these all depend on whether we view an object as a definite fixed sample or as part of a broader population of samples. However, as all statistical models are wrong (McCullagh and Nelder, 1989), and as we will obtain different expectations and uncertainties by varying the properties within the age–depth relationship estimation, all we can say, given the specified properties chosen (polynomial or smoother, AIC or cross-validation, weights of objects), is that this will be the expected age at particular depths, and this is the uncertainty associated with that estimate. To obtain better results we need more information, which leads to our general recommendation of submitting more objects for dating. It is important to remember that with few dates (10–15) the age–depth model statistics will be no more than a guess (Telford *et al.*, 2004b).

Acknowledgements

We would like to thank Oliver Heiri, Andre F. Lotter, Anne E. Bjune, Keith D. Bennett, Eric Grimm, and the NORPEC and HOLIVAR research communities for valuable input and discussions. We also thank the Norwegian Research Council (155875/720) and Bjerknes Centre for Climate Research for

financial support. This is publication no. A94 of Bjerknes Centre of Climate Research.

Appendix 1

To apply the functions `Cagedepth.fun` and `Cagenew.fun` (Heegaard 2003) using the Windows-version of the free statistical software R (<http://cran.r-project.org/>; last accessed 22 February 2005).

- (1) Download and install R from their homepage (windows version).

Open R

- (2) Download and import the `Cagedepth` functions into R (copy the content `CagedepthR.txt` into the R-command window. This version also works under Unix platforms). For Mac users download `CageMac13.txt`.

```
#Copy the depths and calibrated ranges as labelled in Table 1
#from a spreadsheet
> lake.df <- read.table("clipboard",header = T) #imports the
#data into a data.frame in R
> attach(lake.df) #attach the data.frame to the search path
#of R
> library(mgcv) #opens the library mgcv in R (Wood, 2001)
> fit.mod <- Cagedepth.fun(depthup,depthdo,cageup,cagedo)
#Runs a default estimation of the calibrated age depth
#relationship. This generates two
#plots (Figures 2 and 3), and a numerical output to the object
#fit.mod (extracts in Table 2).
#For more information on modelling options see.
#http://www.bio.uu.nl/~palaeo/Congressen/Holivar/
#Literature_Holivar2003.htm (last accessed 22 February 2005).
#The Cagedepth.fun function takes the arguments depthup,
#depthdo, cageup, cagedo,
#weights, vspan, and k. The first four arguments describe the
#characteristics of the dated
#objects, the weights argument is a vector of length n that
#specifies the weights to be
#used in the weighted regression (default is 1 for the top layer
#and 1/sd from the
#calibrated uncertainty, note that 0 = 1/sd), the vspan
#(default = 1) is a parameter of
#the local regression used in the diagnostic plot (reduced
#increase roughness), and k is
#a number of splines used in the cubic smooth spline
#regression (default k = n - 1, this can not exceed n, and lower
#k can reduce roughness in the estimated age–depth
#relationship).
> fit1.mod <-
Cagedepth.fun(depthup,depthdo,cageup,cagedo,weights =
rep(1,length(depthup)),vspan = 0.8, k = 5)
#This models the age–depth relationship by equal weight for
#all dated objects, the
#diagnostic plot local regression has a span of 0.8, and we have
#used five basis functions #in the smooth spline algorithm.
#The following R commands will export data as comma
#separated text-files for #producing Table 2.
> write.table(fit.mod$Constant,file = "const.csv",sep = ",")
> write.table(fit.mod$Muvar,file = "muvar.csv",sep = ",")
```

```
#Estimations for new depths through the core
> fit.new <- Cagenew.fun(fit.mod,1,1:360)
#This function estimates ages and their 95% confidence
interval by using the object
#fit.mod, with 1 = constant variance (optional 2 =  $\mu$  variance),
for each centimetre between #1 and 360.
```

References

- Appleby, P.G. 2001: Chronostratigraphic techniques in recent sediments. In Last, W.M. and Smol, J.P., editors, *Tracking environmental change using lake sediments volume 1: basin analysis, coring, and chronological techniques*. Dordrecht: Kluwer Academic Publishers, 171–203.
- Bennett, K.D. 1994: Confidence intervals for age estimates and deposition times in late-Quaternary sediment sequences. *The Holocene* 4, 337–48.
- Bennett, K.D. and Fuller, J.L. 2002: Determining the age of the mid-Holocene *Tsuga canadensis* (hemlock) decline, eastern North America. *The Holocene* 12, 421–29.
- Bigler, C., Larocque, I., Peglar, S.M., Birks, H.J.B. and Hall, R.I. 2002: Quantitative multiproxy assessment of long-term patterns of Holocene environmental change from a small lake near Abisko, northern Sweden. *The Holocene* 12, 481–96.
- Boaretto, E., Bryant, C., Carmi, I., Cook, G., Harkness, D., Heinemeier, J., McClure, J., McGee, E., Naysmith, P., Possnert, G., Scott, M., van der Plicht, H. and van Strydonck, M. 2002: Summary findings of the fourth international radiocarbon intercomparison (FIRI) (1998–2001). *Journal of Quaternary Science* 17, 633–37.
- Boreux, J.-J., Pesti, G., Duckstein, L. and Nicolas, J. 1997: Age model estimation in paleoclimatic research: fuzzy regression and radiocarbon uncertainties. *Palaeogeography, Palaeoclimatology, Palaeoecology* 128, 29–37.
- Brauer, A., Litt, T., Negendank, J.F.W. and Zolitschka, B. 2001: Lateglacial varve chronology and biostratigraphy of lakes Holzmaar and Meerfelder Maar, Germany. *Boreas* 30, 83–88.
- Buck, C.E., Cavanagh, W.G. and Litton, C.D. 1996: *Bayesian approach to interpreting archaeological data*. Chichester: Wiley.
- Firth, D. 1991: Generalized linear models. In Hinkley, D.V., Reid, N. and Snell, E.J., editors, *Statistical theory and modelling, in honour of Sir David Cox, FRS*. London: Chapman & Hall, 55–82.
- Hastie, T.J. and Tibshirani, R.J. 1990: *Generalized additive models*. London: Chapman and Hall.
- Hastie, T., Tibshirani, R. and Friedman, J. 2001: *The elements of statistical learning*. New York: Springer.
- Heegaard, E. 2003: Mixed effect age–depth routine for R. Retrieved 26 January 2005 from http://www.bio.uu.nl/~palaeo/Congressen/Holivar/Literature_Holivar2003.htm or <http://www.uib.no/bot/qeprg/Age-depth.htm>
- Heiri, O., Lotter, A.F., Hausmann, S. and Kienast, F. 2003a: A chironomid-based Holocene summer air temperature reconstruction from the Swiss Alps. *The Holocene* 13, 477–84.
- Heiri, O., Wick, L., van Leeuwen, J.F.N., van der Knaap, W.O. and Lotter, A.F. 2003b: Holocene tree immigration and the chironomid fauna of a small Swiss subalpine lake (Hinterburgsee, 1515 m asl). *Palaeogeography, Palaeoclimatology, Palaeoecology* 189, 35–53.
- Maher, L.J., Jr 1972: Absolute pollen diagram of Redrock Lake, Boulder County, Colorado. *Quaternary Research* 2, 531–53.
- McCullagh, P. and Nelder, J.A. 1989: *Generalized linear models*. 2nd edition. London: Chapman & Hall.
- Myers, R.H., Montgomery, D.C. and Vining, G.G. 2002: *Generalized linear models*. New York: John Wiley & Sons.
- Pinheiro, J.C. and Bates, D.M. 2000: *Mixed-effects models in S and S-plus*. New York: Springer.
- Ramsey, C.B. 2001: Development of the radiocarbon calibration program. *Radiocarbon* 43, 355–63.
- Rosén, P., Segerström, U., Eriksson, L., Renberg, I. and Birks, H.J.B. 2001: Holocene climatic change reconstructed from diatoms, chironomids, pollen and near-infrared spectroscopy at an alpine lake (Sjuodjijaure) in northern Sweden. *The Holocene* 11, 551–62.
- Seppä, H. and Birks, H.J.B. 2001: July mean temperature and annual precipitation trends during the Holocene in the Fennoscandian tree-line area: pollen-based reconstructions. *The Holocene* 11, 527–39.
- 2002: Holocene climate reconstructions from the Fennoscandian tree-line area based on pollen data from Toskäljavri. *Quaternary Research* 57, 191–99.
- Seppä, H., Nyman, M., Korhola, A. and Weckström, J. 2002: Changes of treelines and alpine vegetation in relation to post-glacial climate dynamics in northern Fennoscandia based on pollen and chironomid records. *Journal of Quaternary Science* 17, 287–301.
- Stuiver, M. and Reimer, P.J. 1993: Extended C-14 data-base and revised CALIB 3.0 C-14 age calibration program. *Radiocarbon* 35, 215–30.
- Telford, R.J., Heegaard, E. and Birks, H.J.B. 2004a: The intercept is a poor estimate of a calibrated radiocarbon age. *The Holocene* 14, 296–98.
- 2004b: Validation of age–depth modelling techniques using simulated radiocarbon dates on varved sediments. *Quaternary Science Reviews* 23, 1–5.
- Venables, W.N. and Ripley, B.D. 2002: *Modern applied statistics with S*. 4th edition. New York: Springer.
- Wood, S.N. 2000: Modelling and smoothing parameter estimation with multiple quadratic penalties. *Journal of the Royal Statistical Society, Series B* 62, 413–28.
- 2001: mgcv: GAMs and generalised ridge regression for R. *R News* 1, 20–25.