



*Supplement of*

## **SCUBIDO: a Bayesian modelling approach to reconstruct palaeoclimate from multivariate lake sediment data**

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## Supplementary Information 1: notations and variables used in the approach

Supplementary Table 1: Definitions of variables and model parameters used in the Bayesian framework.

Symbol	Description
$C_i$	Climate variable at time point $i$
$C^m, C^f$	Modern and fossil climate variable vectors
$XRF_{ij}$	Clr-transformed $\mu$ XRF-CS data at depth $i$ and element $j$
$t_i$	Calibrated age (in cal years BP) of depth $i$
$\theta$	Vector of regression parameters ( $\beta_0, \beta_1, \beta_2, \mu_0$ )
$\sigma_c$	Standard deviation of the climate random walk
$\mu_{ij}$	Mean of the multivariate normal distribution for element $j$ at depth $i$
$\Sigma$	Covariance matrix of residuals from the regression
$MVN$	Multivariate normal distribution
$M_i$	Vector of mean values $\mu_{ij}$ across all elements for depth $i$
$\omega_i$	Variance term in the continuous-time random walk, scaled by age spacing
$\beta_0, \beta_1$ , and $\beta_2$	Regression coefficients for element $j$
$MDP$	Marginal Data Posterior (posterior distribution for each time slice)
$\Sigma^{-1} \sim \text{Wishart}(R, k + 1)$	Prior on inverse covariance matrix
$\sigma_c \sim \text{LN}(a, b)$	Log-normal prior on random walk standard deviation

## Supplementary Information 2: mathematical details on the marginal data posterior fitting.

Marginal data posteriors

In order to fit the marginal data posteriors (MDPs) we use the  $\theta$  which was calculated in the calibration stage and introduce the fossil XRF data ( $XRF^f$ ). We use  $k$  MDPs of each time slice as a reference to the sum of each multivariate normal distribution for each of the 11 chemical elements ( $j$ )

$$MDP_{ik} | C_i \sim MVN(\mu_{MDP_i}, prec_{MDP_i})$$

This stage also requires the use of a climate grid which is 50 possible climate values which are placed on a 50 x 50 regular grid. For example, if we were estimating temperature anomalies, the grid may look like a 50-part sequence from -3 °C to +3 °C, or precipitation may look like -100 mm to +100 mm. By having the climate grid helps the model choose sensible climate scenarios.

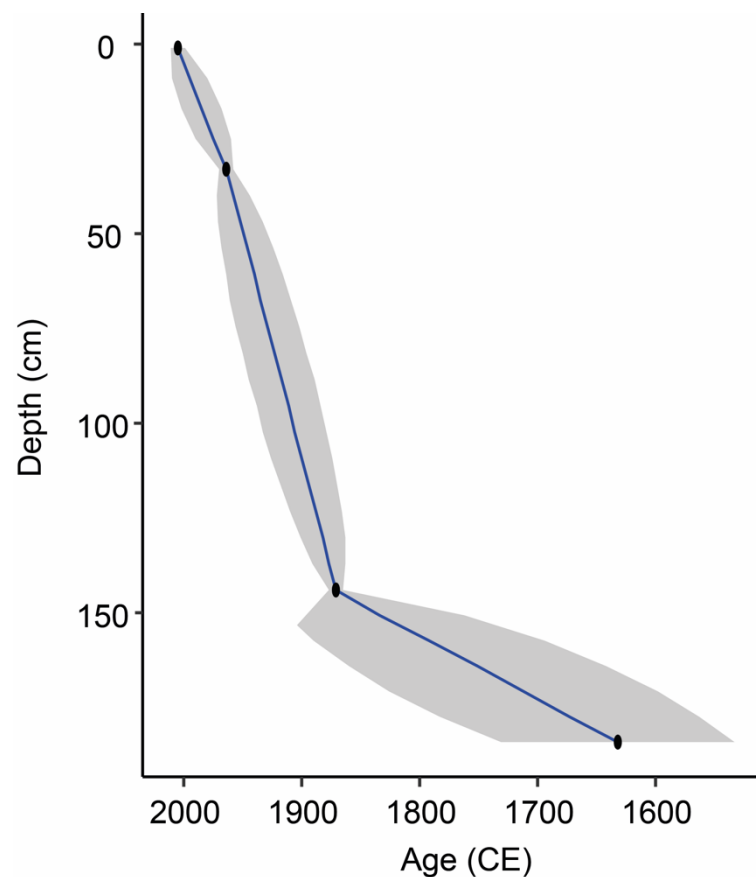
The output of the final MDP calculation is a MDP for each layer of the fossil XRF data which can be used within the final reconstruction of climate through time.

In the walk-through example (Section 4.0 main text), the climate grid chosen for Diss Mere was -3 °C and +3 °C having a range of 6 °C in total which is sufficient to cover the variability in temperatures reconstructed in the Holocene for other studies (Osman et al., 2021).

### **Supplementary Information 3** Diss Mere's non-varved chronology

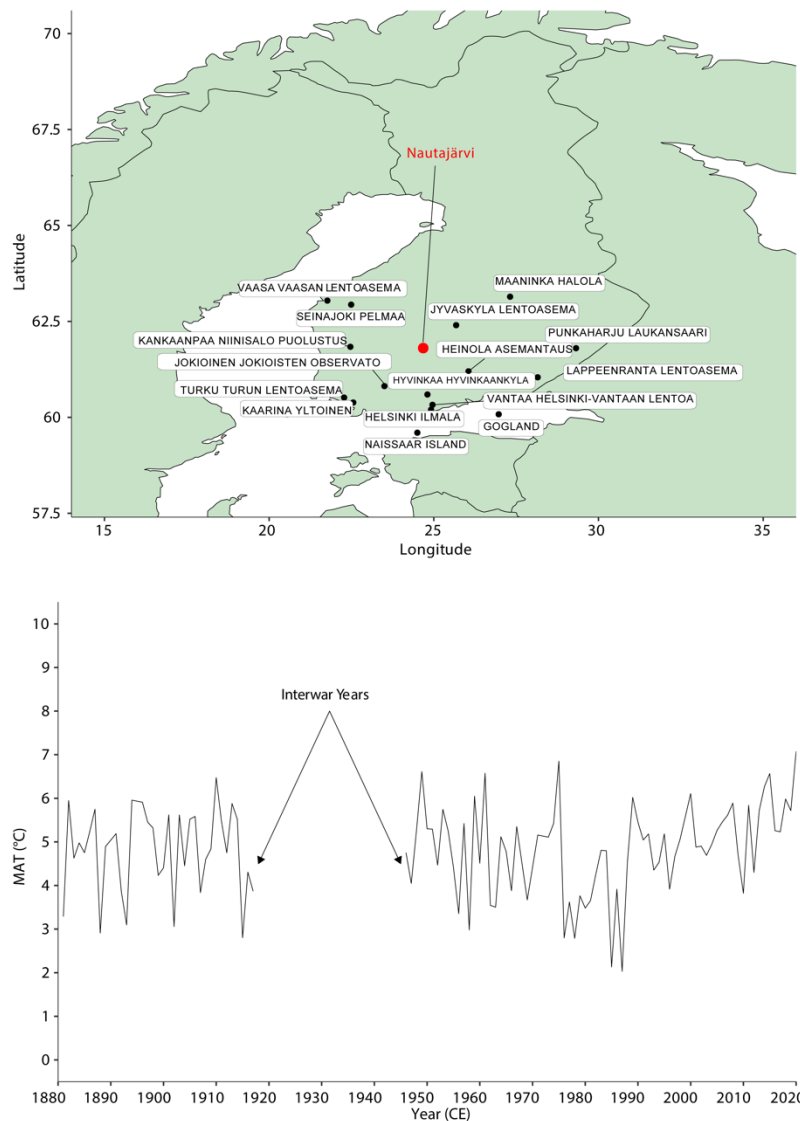
The full chronology and age model for the non-varved sediments is described and

published in Boyall et al. (2024). This is based on a combination of tephra layers that link the non-varved and the varve chronology, radiocarbon dates and the 1963 CE  $^{137}\text{Cs}$  peak. The average age uncertainty for the non-varved section of Diss Mere is  $\pm 65$  years and thus is higher than the varve chronology. During the calibration period (1700 – 1932 CE), the age uncertainty is smaller at the top of the sequence with a maximum uncertainty of  $\pm 22$  years between 1932 CE and 1800 CE, however this increases gradually to  $\pm 110$  years for the following century (Supplementary Figure 1). The sedimentation rate within this period is very high (0.15 cm/year) and includes up to 20 data points per year.



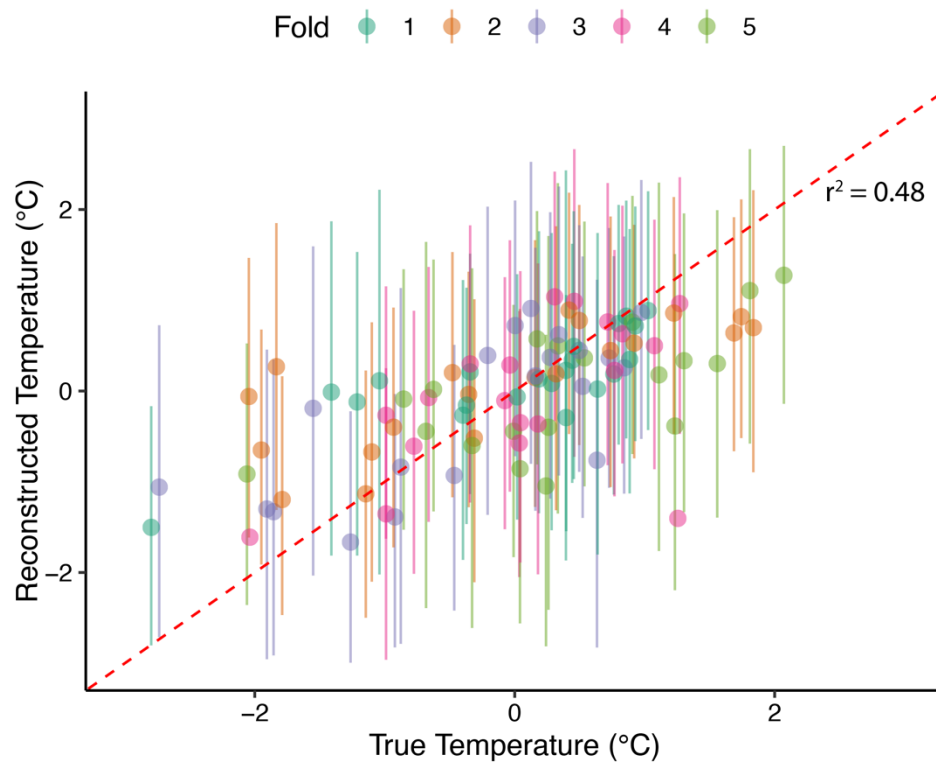
Supplementary Figure 1: Age-depth model for Diss Mere during the calibration period and the full age model for the non-varved section of the Diss Mere sediments can be found in Boyall et al. (2024).

#### Supplementary Information 4: locations of meteorological weather stations for Nautajärvi calibration



Supplementary Figure 2: A figure showing the locations of the weather stations used to build a composite record of annual mean temperatures for Nautajärvi and a timeseries showing the record with an interwar period of no data.

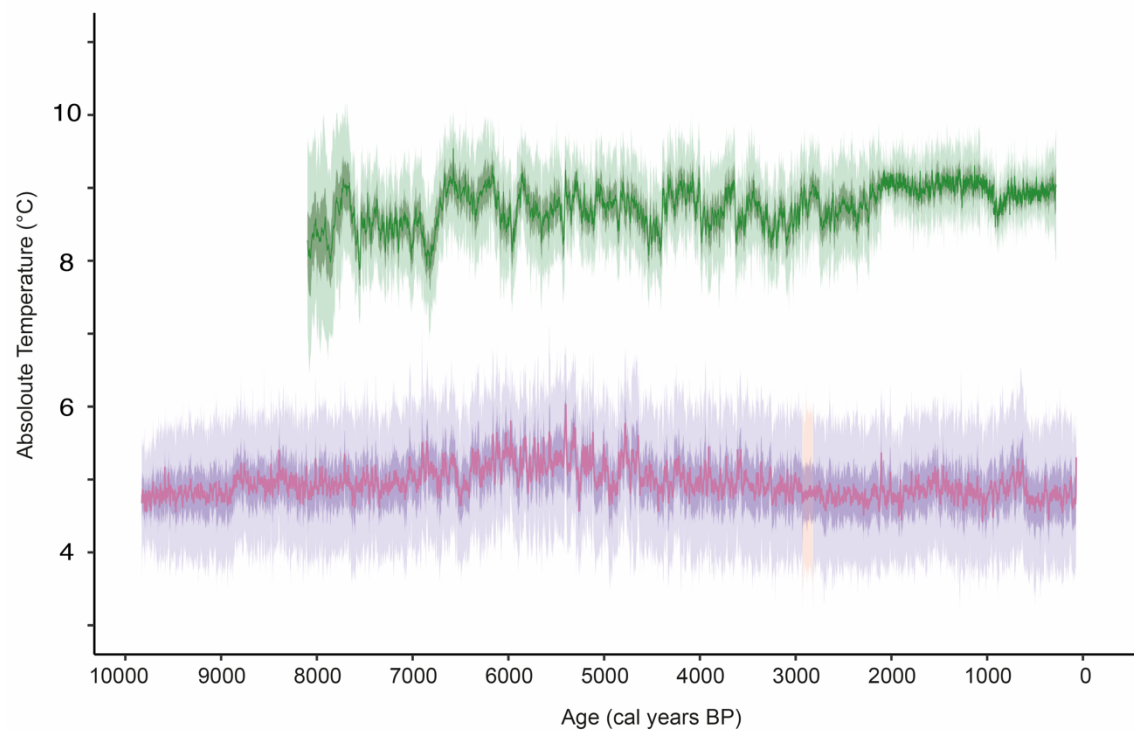
### Supplementary Information 5: Validation results for Nautajärvi.



Supplementary Figure 3: True vs reconstructed temperature for Nautajärvi with the colours dots and bars representing the fold results for the median and confidence intervals, respectively.

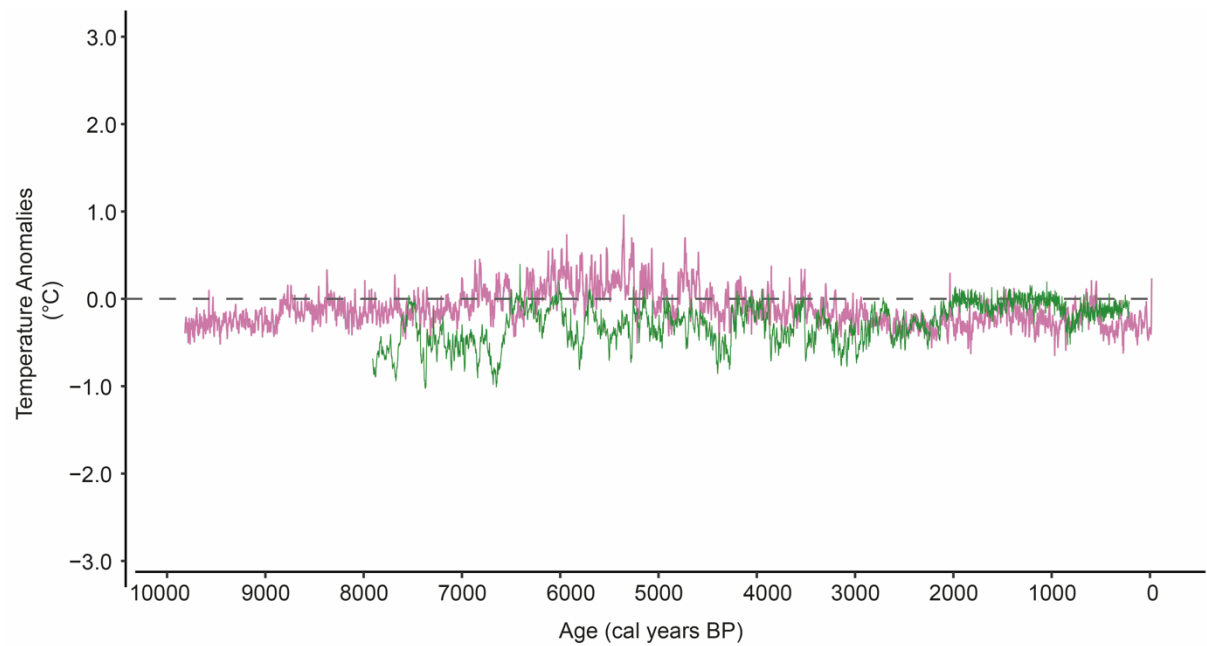
The same out-of-sample validation approach detailed in the main manuscript for Diss Mere was applied on the calibration period for Nautajärvi. The coverage percentage for is 94.95% and the  $r^2$  value is 0.48 ( $P = <0.001$ ).

**Supplementary Information 6:** Absolute temperatures of the Diss Mere and Nautajärvi reconstruction



Supplementary Figure 4: A figure showing the Diss Mere (green) and Nautajärvi (purple) reconstructions in absolute temperatures

## Supplementary Information 7: Diss Mere and Nautajärvi temperature reconstructions



Supplementary Figure 5: Diss Mere (green) and Nautajärvi (purple) reconstructions without uncertainty envelopes. Reference period 1991-2020