Supplementary materials for: Modelling palaeoecological time series using generalized additive models

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1 Introduction

This document is an annotated version of the R code used to fit the GAMs and related analyses to the Small Water and Braya-Sø example data sets.

The following packages are required: *mgcv*, *scam*, *ggplot2*, *cowplot*, and *tidyr*. Also, the *schoenberg* package is required; it is not on CRAN but can be installed from Github.

```
library("mgcv")
```

```
#> Loading required package: nlme
#> This is mgcv 1.8-23. For overview type 'help("mgcv-package")'.
```

```
library("scam")
```

```
#> This is scam 1.2-2.
```

```
library("ggplot2")
library("cowplot")
```

```
#>
#> Attaching package: 'cowplot'
#> The following object is masked from 'package:ggplot2':
#>
#>     ggsave
```

```
## schoenberg is not on CRAN, install from github:
## install.packages("devtools")
## devtools::install_github("gavinsimpson/schoenberg")
library("schoenberg")
library("tidyr")

## Default ggplot theme
theme_set(theme_bw())
```

The example data sets are also stored on github; https://github.com/gavinsimpson/frontiers-palaeo-additive-modelling. Once downloaded the data are read in and processed a little

```
## source Small Water data
small <- readRDS("./data/small-water/small-water-isotope-data.rds")
head(small)
```

```
#>   Depth   d13C  TotalC d15N TotalN DryWeight     Year
#> 1   0.2 -27.57  806.49 3.05  64.21       8.2 2007.254
#> 2   0.4 -27.67  949.33 3.01  73.26       7.6 2006.510
#> 3   0.8 -27.63 1305.52 2.93  93.25      11.6 2004.941
#> 4   1.2 -27.62 1136.04 2.33  86.09       9.6 2003.269
#> 5   1.6 -27.48 1028.27 2.09  93.80      10.9 2001.496
#> 6   2.0 -27.39  809.91 2.66  79.98       9.9 1999.626
```

```
## load braya so data set
braya <- read.table("./data/braya-so/DAndrea.2011.Lake Braya So.txt",
                    skip = 84)
names(braya) <- c("Depth", "DepthUpper", "DepthLower", "Year", "YearYoung",
                  "YearOld", "UK37")
braya <- transform(braya, sampleInterval = YearYoung - YearOld)
head(braya)
```

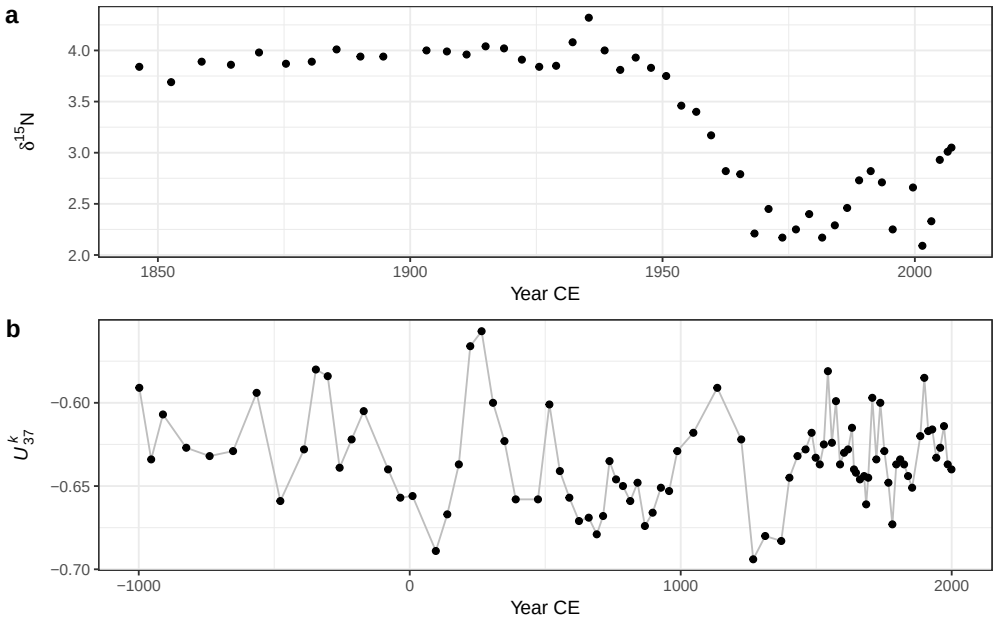
```
#>   Depth DepthUpper DepthLower     Year YearYoung YearOld   UK37
#> 1  0.25        0.0        0.5 1999.125   2006.00 1992.25 -0.640
#> 2  0.75        0.5        1.0 1985.375   1992.25 1978.50 -0.637
#> 3  1.25        1.0        1.5 1971.525   1978.50 1964.55 -0.614
#> 4  1.75        1.5        2.0 1957.575   1964.55 1950.60 -0.627
#> 5  2.25        2.0        2.5 1943.150   1950.60 1935.70 -0.633
#> 6  2.75        2.5        3.0 1928.250   1935.70 1920.80 -0.616
#>   sampleInterval
#> 1          13.75
#> 2          13.75
#> 3          13.95
#> 4          13.95
#> 5          14.90
#> 6          14.90
```

```
## plot labels
d15n_label <- expression(delta^{15}*N)
braya_ylabel <- expression(italic(U)[37]^{italic(k)})
```

Plots of the two data sets are prepared using *ggplot2*

```
## plot Small Water data
small_plt <- ggplot(small, aes(x = Year, y = d15N)) +
    geom_point() +
```

```
    labs(y = d15n_label, x = "Year CE")

## Generate a plot of the data
braya_plt <- ggplot(braya, aes(x = Year, y = UK37)) +
    geom_line(colour = "grey") +
    geom_point() +
    labs(y = braya_ylabel, x = "Year CE")

## Recreate plot from manuscript
plot_grid(small_plt, braya_plt, ncol = 1, labels = "auto", align = "hv",
          axis = "lr")
```



2 Fitting GAMs

The GAM plus CAR(1) process is fitted to the Small Water data set using the `gamm()` function. This fits GAMs as mixed effects models via the *nlme* package, which allows the use of correlation structures in the model residuals via the `correlation` argument. Here, the `corCAR1()` function is used to select the CAR(1) process and we specify the ordering of samples via the `Year` variable in `small`.

```
## fit small water GAM usin gamm() with a CAR(1)
mod <- gamm(d15N ~ s(Year, k = 15), data = small,
            correlation = corCAR1(form = ~ Year), method = "REML")
```

The estimated value of ϕ for the CAR(1) can be extracted from the fitted model via the `$lme` component. Here we just extract the correlation structure component.

```
## estimate of phi and confidence interval
smallPhi <- intervals(mod$lme, which = "var-cov")$corStruct
smallPhi
```

```
#>         lower      est.     upper
#> Phi 0.2811107 0.6026967 0.8547543
#> attr(,"label")
#> [1] "Correlation structure:"
```

The model summary is prepared from the $gam component of the fitted model

```
## summary object
summary(mod$gam)
```

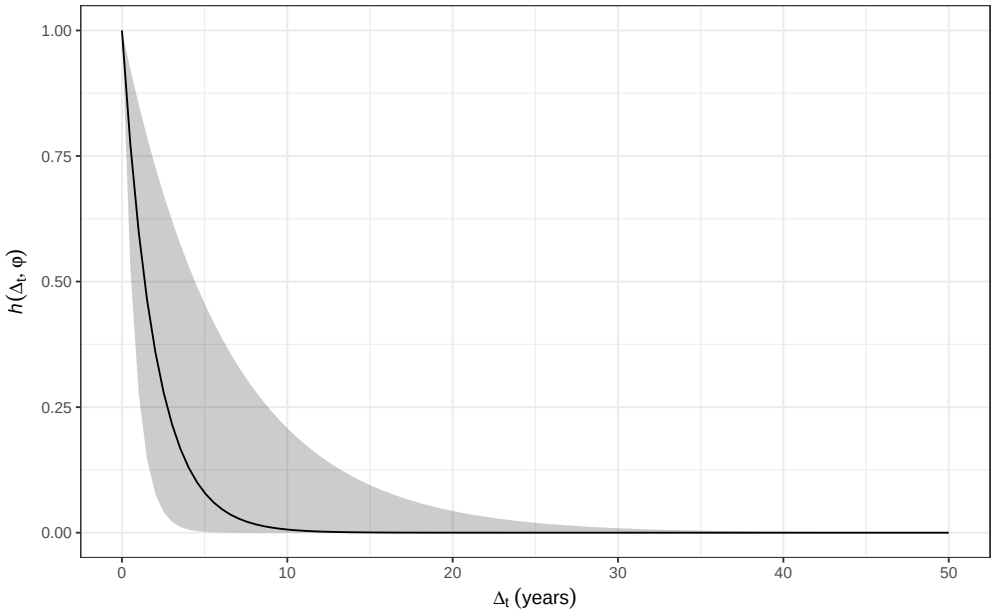
```
#>
#> Family: gaussian
#> Link function: identity
#>
#> Formula:
#> d15N ~ s(Year, k = 15)
#>
#> Parametric coefficients:
#>             Estimate Std. Error t value Pr(>|t|)
#> (Intercept)  3.30909    0.03489   94.84   <2e-16 ***
#> ---
#> Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
#>
#> Approximate significance of smooth terms:
#>           edf Ref.df     F p-value
#> s(Year) 7.954  7.954 47.44  <2e-16 ***
#> ---
#> Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
#>
#> R-sq.(adj) =  0.929
#>   Scale est. = 0.037268  n = 48
```

The output shows the estimated complexity of the fitted smooth, in terms of the effective degrees of freedom of the spline. An associated F statistic and test of the null hypothesis of no trend (effect). Here the estimated trend provides strong evidence against this null.

The CAR(1) process plotted in Figure 10 of the manuscript was prepared using

```
## plot CAR(1) process
maxS <- with(small, diff(range(Year))) ## too large, truncate to 50
S <- seq(0, 50, length = 100)

car1 <- setNames(as.data.frame(t(outer(smallPhi, S, FUN = `^`)[1, , ])),
```

```
                  c("Lower","Correlation","Upper"))
car1 <- transform(car1, S = S)

car1Plt <- ggplot(car1, aes(x = S, y = Correlation)) +
    geom_ribbon(aes(ymax = Upper, ymin = Lower),
                fill = "black", alpha = 0.2) +
    geom_line() +
    ylab(expression(italic(h) * (list(Delta[t], varphi)))) +
    xlab(expression(Delta[t] ~ (years)))
car1Plt
```



The exponential decline in correlation with increasing separation is evident here; once samples are ~10 years apart, there is little estimated dependence between them.

The same model is fitted to the Braya-Sø data set. Note however that in order to even fit the model with both a smooth and the CAR(1) process, I have had to change the default optimiser used to fit the model, and reduce the basis dimension to a small number. We also fit the model using GCV, which is the defaut, hence no `method` argument

```
## fit the car(1) model --- needs optim as this is not a stable fit!
## also needs k setting lower than default
braya.car1 <- gamm(UK37 ~ s(Year, k = 5), data = braya,
                   correlation = corCAR1(form = ~ Year),
                   method = "REML",
                   control = list(niterEM = 0, optimMethod = "BFGS",
                                  opt = "optim"))

## fit model using GCV
braya.gcv <- gam(UK37 ~ s(Year, k = 30), data = braya)
```

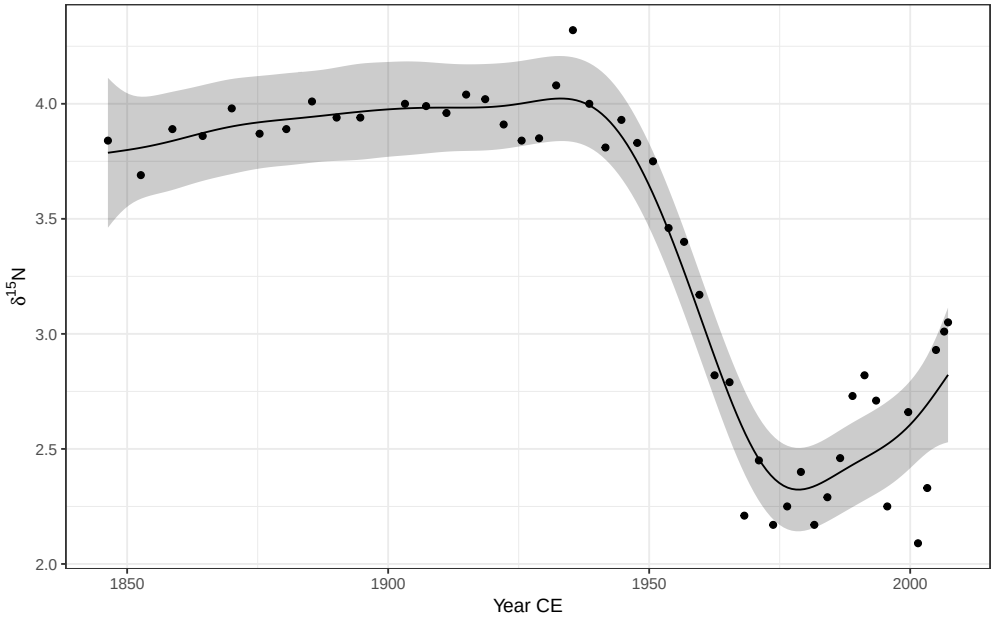
```
## estimate of phi and confidence interval
brayaPhi <- intervals(braya.car1$lme)$corStruct
brayaPhi
```

```
#>            lower      est. upper
#> Phi 1.611049e-22 0.2000156     1
#> attr(,"label")
#> [1] "Correlation structure:"
```

Note the wide confidence interval — effectively 0–1 — on ϕ. If you were to increase the value of `k` to be `k = 10` in the `s(Year)` above, the model will fit but a warning message will be emitted when trying to extract ϕ due to a non-positive definite model covariance matrix, indicating problems with the model.

The next couple of code chunks prepare plots of the fitted GAMS. The general idea is to predict fom the fitted model for a fine grid of points over the range of the time variable. First we plot the trend for Small Water with an approximate 95% confidence interval assuming asymptotic normality

```
N <- 300   # number of points at which to evaluate the splines
## Predict from the fitted model
newYear <- with(small, data.frame(Year = seq(min(Year), max(Year),
                                             length.out = 200)))
newYear <- cbind(newYear,
                 data.frame(predict(mod$gam, newYear, se.fit = TRUE)))
newYear <- transform(newYear,
                     upper = fit + (2 * se.fit),
                     lower = fit - (2 * se.fit))

## Plot simulated trends
small_fitted <- ggplot(newYear, aes(x = Year, y = fit)) +
    geom_ribbon(aes(ymin = lower, ymax = upper, x = Year), alpha = 0.2,
                inherit.aes = FALSE, fill = "black") +
    geom_point(data = small, mapping = aes(x = Year, y = d15N),
               inherit.aes = FALSE) +
    geom_line() +
    labs(y = d15n_label, x = "Year CE")
small_fitted
```



For Braya-Sø, we repeat the process, but we do so for both models (GAMM + CAR(1) and GCV), and use a critical value from the t distribution to form the confidence interval

```
## ggplot with data and fitted spline, then resids vs time in second panel
newBraya <- with(braya, data.frame(Year = seq(min(Year), max(Year),
                                              length.out = N)))
newBraya <- cbind(newBraya,
                  data.frame(predict(braya.car1$gam, newBraya,
                                     se.fit = TRUE)))
crit.t <- qt(0.975, df = df.residual(braya.car1$gam))
newBraya <- transform(newBraya,
                      upper = fit + (crit.t * se.fit),
                      lower = fit - (crit.t * se.fit))
## add GAM GCV results
fit_gcv <- predict(braya.gcv, newdata = newBraya, se.fit = TRUE)
newBraya <- rbind(newBraya, newBraya) # extend newBraya to take GCV results
newBraya[seq(N+1, length.out = N, by = 1), ]$fit <- fit_gcv$fit
newBraya[seq(N+1, length.out = N, by = 1), ]$upper <-
    fit_gcv$fit + (qt(0.975, df.residual(braya.gcv)) * fit_gcv$se.fit)
newBraya[seq(N+1, length.out = N, by = 1), ]$lower <-
    fit_gcv$fit - (qt(0.975, df.residual(braya.gcv)) * fit_gcv$se.fit)
newBraya <- transform(newBraya,
                      Method = rep(c("GAMM (CAR(1))", "GAM (GCV)"),
                                   each = N))

## plot CAR(1) and GCV fits
braya_fitted <- ggplot(braya, aes(y = UK37, x = Year)) +
    geom_point() +
```

```
    geom_ribbon(data = newBraya,
                mapping = aes(x = Year, ymax = upper, ymin = lower,
                              fill = Method),
                alpha = 0.3, inherit.aes = FALSE) +
    geom_line(data = newBraya,
              mapping = aes(y = fit, x = Year, colour = Method)) +
    labs(y = braya_ylabel, x = "Year CE") +
    scale_color_manual(values = c("#5e3c99", "#e66101")) +
    scale_fill_manual(values = c("#5e3c99", "#e66101")) +
    theme(legend.position = "right")
braya_fitted
```

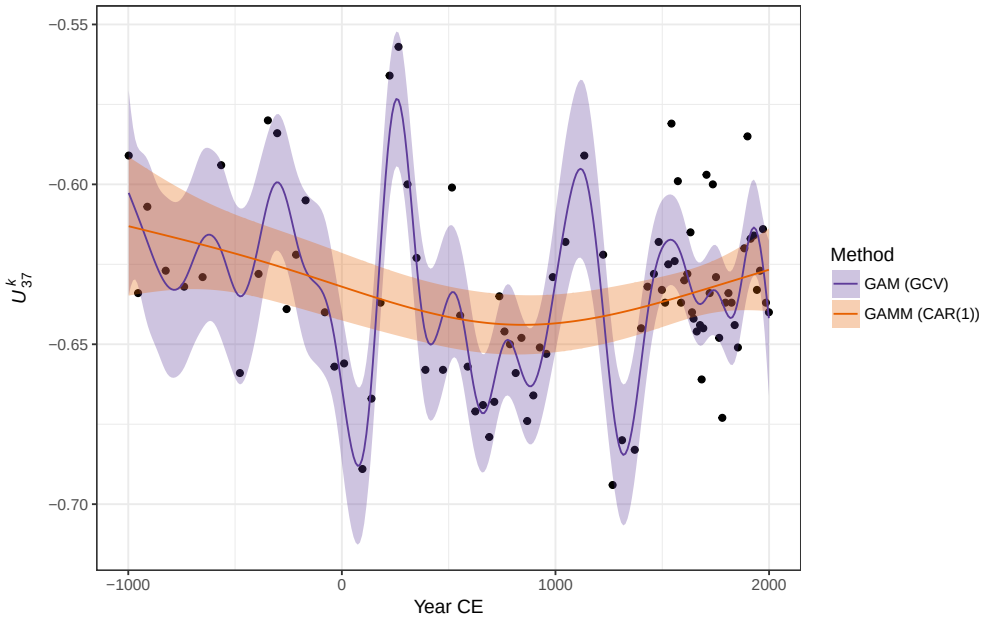
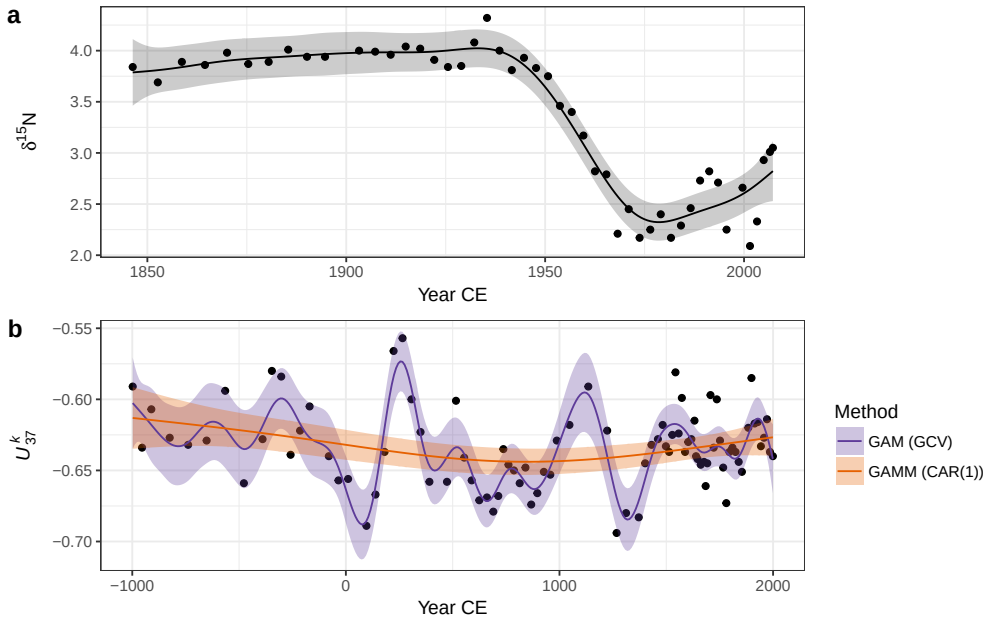


Figure 5 in the manuscript was produced using:

```
plot_grid(small_fitted, braya_fitted, ncol = 1, labels = "auto",
          align = "hv", axis = "lr")
```



To proceed with the Braya-Sø example, we need to increase the basis dimension (`k = 45`), fit using `method = "REML"`, and use observational weights. Here I use the `sampleInterval` variable as the measure of lake years per sample, and to avoid changing the model likelihood, the weights are actually the values of `sampleInterval` divided by the mean of `sampleInterval`:

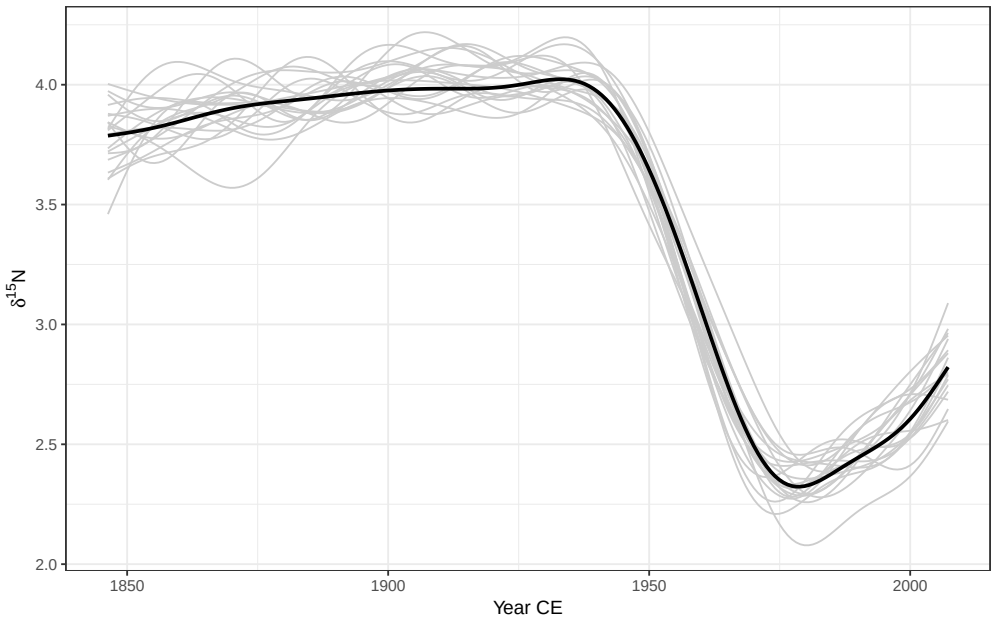
```
## TPRS, weights as sampleInterval
braya_reml <- gam(UK37 ~ s(Year, k = 45, bs = "tp"), data = braya,
                  method = "REML",
                  weights = sampleInterval / mean(sampleInterval))
```

3 Posterior simulation

Samples from the posterior distribution of a GAM can be drawn using the `simulate()` methods from the *schoenberg* package.

```
set.seed(1) # set the random seed to make this reproducible
nsim <- 20  # how many simulations to draw

## do the simulations
sims <- simulate(mod, nsim = nsim, newdata = newYear, unconditional = TRUE)

## rearrange the output into a long/tidy format
colnames(sims) <- paste0("sim", seq_len(nsim))
sims <- setNames(stack(as.data.frame(sims)), c("simulated", "run"))
sims <- transform(sims, Year = rep(newYear$Year, nsim),
                  simulated = simulated)
```

```
## Plot simulated trends
smallSim.plt <- ggplot(newYear, aes(x = Year, y = fit)) +
    geom_line(data = sims,
              mapping = aes(y = simulated, x = Year, group = run),
              colour = "grey80") +
    geom_line(lwd = 1) +
    labs(y = d15n_label, x = "Year CE")
smallSim.plt
```



We repeat the same simulation for Braya-Sø

```
## posterior simulation
## need to reset-up newBraya
newBraya <- with(braya,
                 data.frame(Year = seq(min(Year), max(Year),
                                       length.out = N)))
braya_pred <- cbind(newBraya,
                    data.frame(predict(braya_reml, newBraya,
                                       se.fit = TRUE)))

## simulate
set.seed(1)
sims2 <- simulate(braya_reml, nsim = nsim, newdata = newBraya,
                  unconditional = TRUE)
colnames(sims2) <- paste0("sim", seq_len(nsim))
sims2 <- setNames(stack(as.data.frame(sims2)),
                  c("simulated", "run"))
sims2 <- transform(sims2, Year = rep(newBraya$Year, nsim),
```

```
                        simulated = simulated)

brayaSim.plt <- ggplot(braya_pred, aes(x = Year, y = fit)) +
    geom_line(data = sims2,
              mapping = aes(y = simulated, x = Year, group = run),
              colour = "grey80") +
    geom_line(lwd = 1) +
    labs(y = braya_ylabel, x = "Year CE")
brayaSim.plt
```

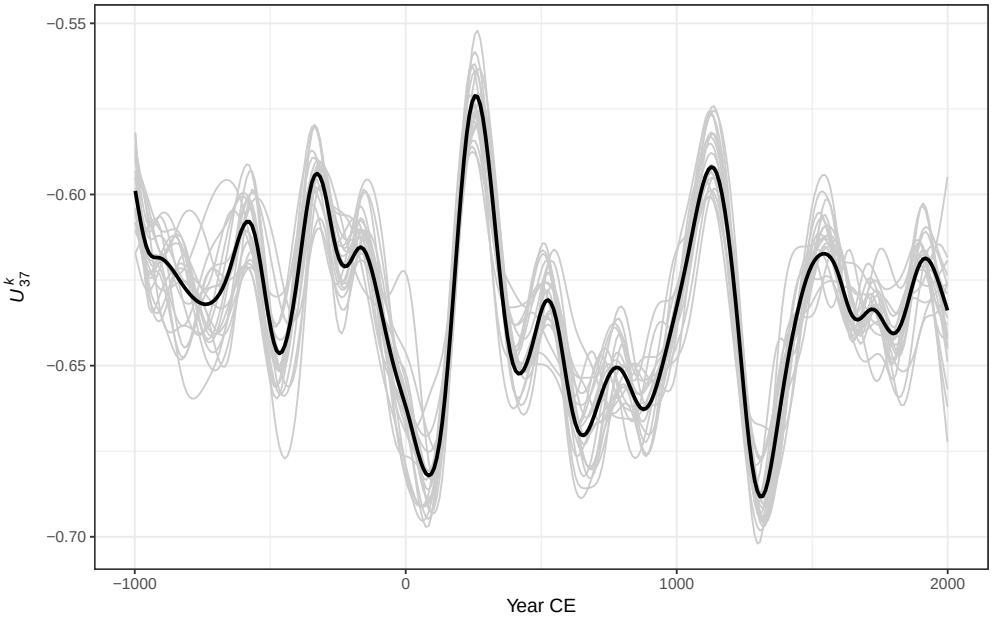
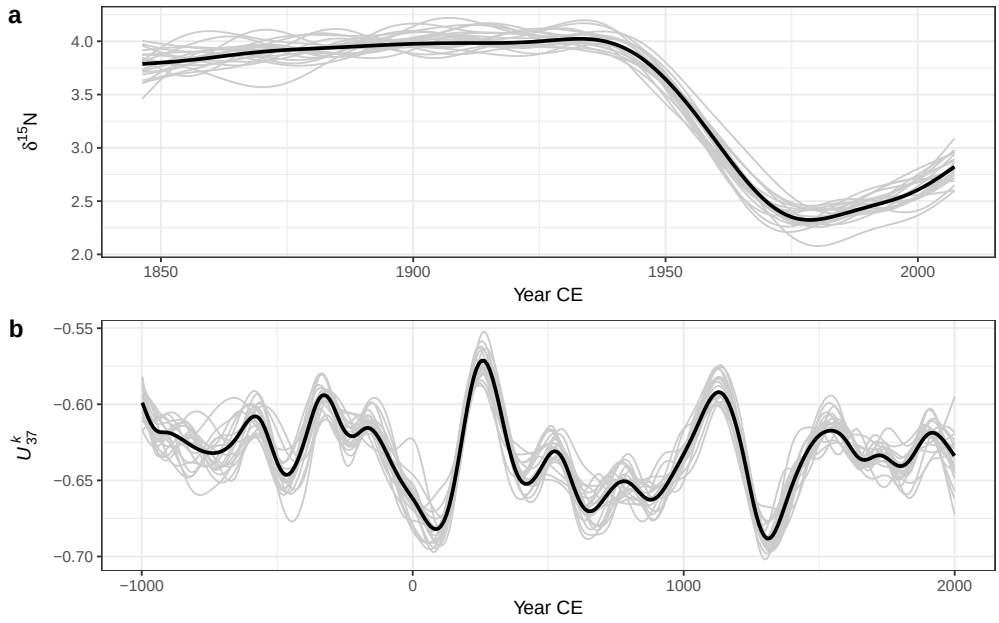


Figure 7 in the manuscript was prepared using

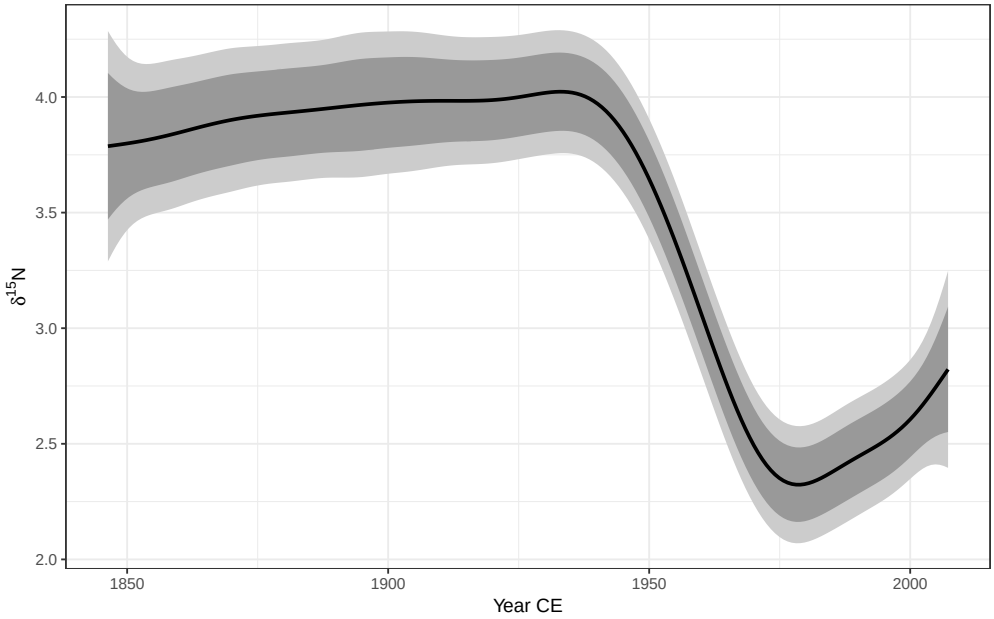
```
plot_grid(smallSim.plt, brayaSim.plt, ncol = 1, labels = "auto",
          align = "hv", axis = "lr")
```



4 Confidence and simultaneous intervals

Across-the-function and simultaneous confidence intervals are computed using the `confint()` method. The type of interval required is given via the `type` argument with options `"confidence"` and `"simultaneous"`.

```
## small water
sw.cint <- confint(mod, parm = "Year", newdata = newYear,
                   type = "confidence")
sw.sint <- confint(mod, parm = "Year", newdata = newYear,
                   type = "simultaneous")

smallInt.plt <- ggplot(sw.cint, aes(x = Year, y = est)) +
    geom_ribbon(data = sw.sint,
                mapping = aes(ymin = lower, ymax = upper, x = Year),
                fill = "grey80", inherit.aes = FALSE) +
    geom_ribbon(mapping = aes(ymin = lower, ymax = upper, x = Year),
                fill = "grey60", inherit.aes = FALSE) +
    geom_line(lwd = 1) +
    labs(y = d15n_label, x = "Year CE")
smallInt.plt
```



124

```
## braya so
bs.cint <- confint(braya_reml, parm = "Year", newdata = newBraya,
                   type = "confidence")
bs.sint <- confint(braya_reml, parm = "Year", newdata = newBraya,
                   type = "simultaneous")

brayaInt.plt <- ggplot(bs.cint, aes(x = Year, y = est)) +
    geom_ribbon(data = bs.sint,
                mapping = aes(ymin = lower, ymax = upper, x = Year),
                fill = "grey80", inherit.aes = FALSE) +
    geom_ribbon(mapping = aes(ymin = lower, ymax = upper, x = Year),
                fill = "grey60", inherit.aes = FALSE) +
    geom_line(lwd = 1) +
    labs(y = braya_ylabel, x = "Year CE")
brayaInt.plt
```

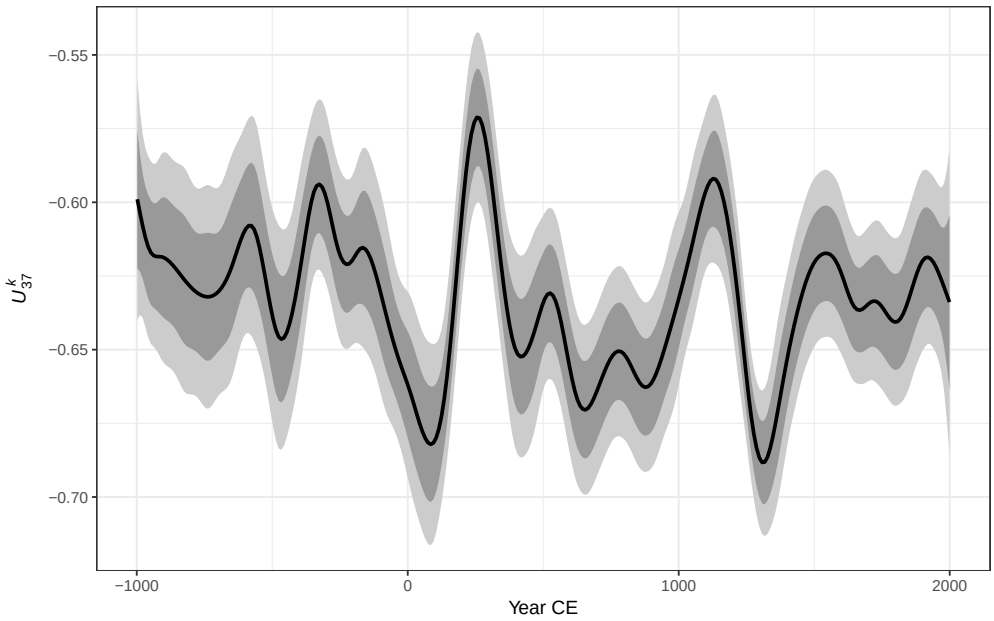
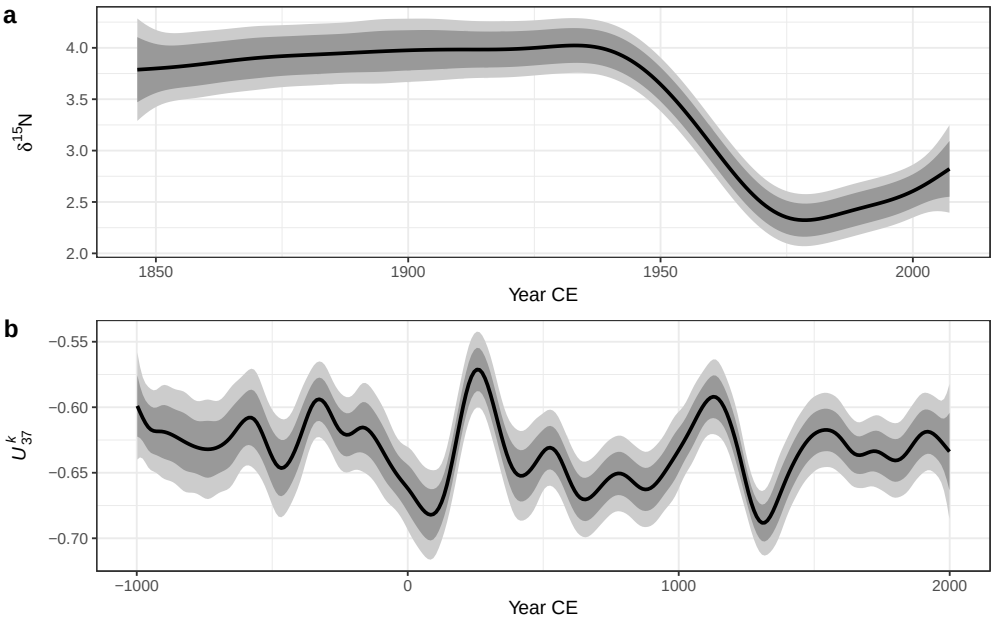


Figure 8 in the manuscript was prepared using

```
plot_grid(smallInt.plt, brayaInt.plt, ncol = 1, labels = "auto",
          align = "hv", axis = "lr")
```



5 Derivatives of the estimated trend

The first derivative of the estimated trend is calculated using finite differences using the `fderiv()` function. There is also a `confint()` method for objects produced by `fderiv()`. The

first derivatives and a 95% simultaneous confidence interval for the Small Water trend we computed and plotted using

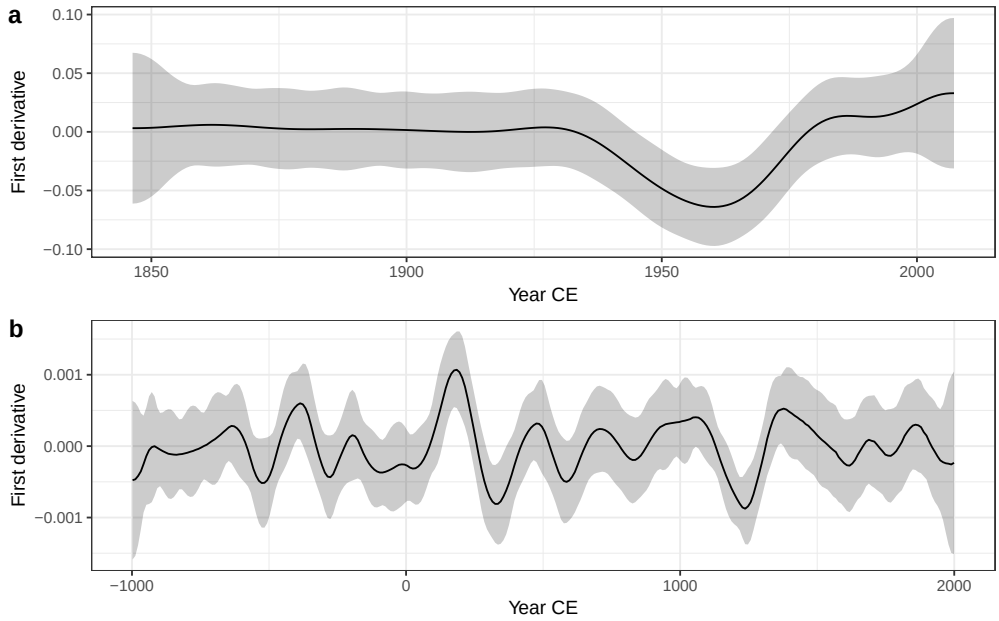
```
small.d <- fderiv(mod, newdata = newYear, n = N)
small.sint <- with(newYear,
                   cbind(confint(small.d, nsim = nsim,
                                 type = "simultaneous"),
                         Year = Year))

small_deriv_plt <- ggplot(small.sint, aes(x = Year, y = est)) +
    geom_ribbon(aes(ymin = lower, ymax = upper), alpha = 0.2,
                fill = "black") +
    geom_line() +
    labs(x = "Year CE", y = "First derivative")
```

whilst for Braya-Sø, the following was used

```
braya.d <- fderiv(braya_reml, newdata = newBraya, n = N)
braya.sint <- with(newBraya,
                   cbind(confint(braya.d, nsim = nsim,
                                 type = "simultaneous"),
                         Year = Year))

braya_deriv_plt <- ggplot(braya.sint, aes(x = Year, y = est)) +
    geom_ribbon(aes(ymin = lower, ymax = upper),
                alpha = 0.2, fill = "black") +
    geom_line() +
    labs(x = "Year CE", y = "First derivative")
```

Figure 9 in the manuscript was prepared using

```
plot_grid(small_deriv_plt, braya_deriv_plt, ncol = 1, labels = "auto",
          align = "hv", axis = "lr")
```



6 Gaussian process smooths

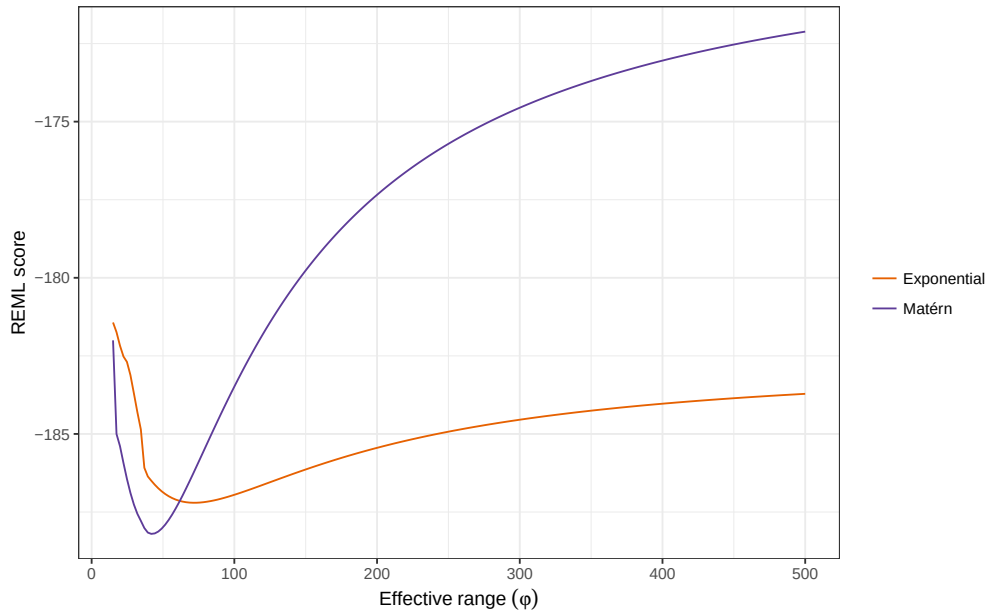
For the Gaussian process smooth to fit within the GAM framework described in the manuscript, we need to supply the value of ϕ for the effective range of the correlation function. To estimate ϕ, we need to repeatedly fit the required GAM using a range of plausible values for ϕ, which we do using a loop. In the chunk below I fit 200 models with ϕ in the range 15–500. For value of ϕ I fit the required GAM and extract the REML score (from component `gcv.ubre`) and store it in the numeric vectors `Mat` or `SEx`, for Matérn and Squared Exponential correlation functions, respectively. The final line of the chunk prepares the REML scores for the two correlation functions in long or tidy format suitable for plotting with *ggplot2*.

```
nn <- 200    # number of points at which to evaluate profile likelihood
dseq <- seq(15, 500, length.out = nn)  # effective ranges to fit at
Mat <- SEx <- numeric(length = nn)     # object to hold model fits
for (i in seq_along(dseq)) {
    ## iterate over dseq, fit GP GAM w Matérn covariance
    Mat[i] <- gam(UK37 ~ s(Year, k = 45, bs = "gp", m = c(3, dseq[i])),
                  weights = sampleInterval / mean(sampleInterval),
                  data = braya, method = "REML",
                  family = gaussian())[["gcv.ubre"]]
    ## fit squared exponential
    SEx[i] <- gam(UK37 ~ s(Year, k = 45, bs = "gp", m = c(2, dseq[i], 1)),
                  weights = sampleInterval / mean(sampleInterval),
                  data = braya, method = "REML",
                  family = gaussian())[["gcv.ubre"]]
}
```

```
## extract the REML score into ggplot-friendly object
reml.scr <- data.frame(cor = rep(c("Matérn","Exponential"), each = nn),
                       effrange = rep(dseq, 2),
                       reml = c(Mat, SEx))
```

The REML scores for the models are plotted with *ggplot2* using

```
## profile-likelihood plot
proflik.plt <- ggplot(reml.scr, aes(x = effrange, y = reml, colour = cor)) +
    geom_line() +
    scale_colour_manual(name = "", values = c("#e66101","#5e3c99")) +
    labs(y = "REML score", x = expression(Effective ~ range ~ (varphi)))
proflik.plt
```



Next we extract the minimum of the REML scores for the two correlation functions and refit those models (we threw away all the models in the `for ()` loop earlier to avoid storing lots of model objects). Then we fit GAMs with Gaussian process smooths using the values of ϕ that produced the minimum REML scores, and predict using the fitted models to visualize the trends.

```
effRange1 <- 250      # sets effective range in years for Matérn correl
## minima from profile likelihood
effRange2 <- with(subset(reml.scr, cor == "Matérn"), dseq[which.min(reml)])
effRange3 <- with(subset(reml.scr, cor == "Exponential"), dseq[which.min(reml)])

## Matern
gp2 <- gam(UK37 ~ s(Year, k = 45, bs = "gp", m = c(3, effRange2)),
           data = braya,
           method = "REML", weights = sampleInterval / mean(sampleInterval))
```

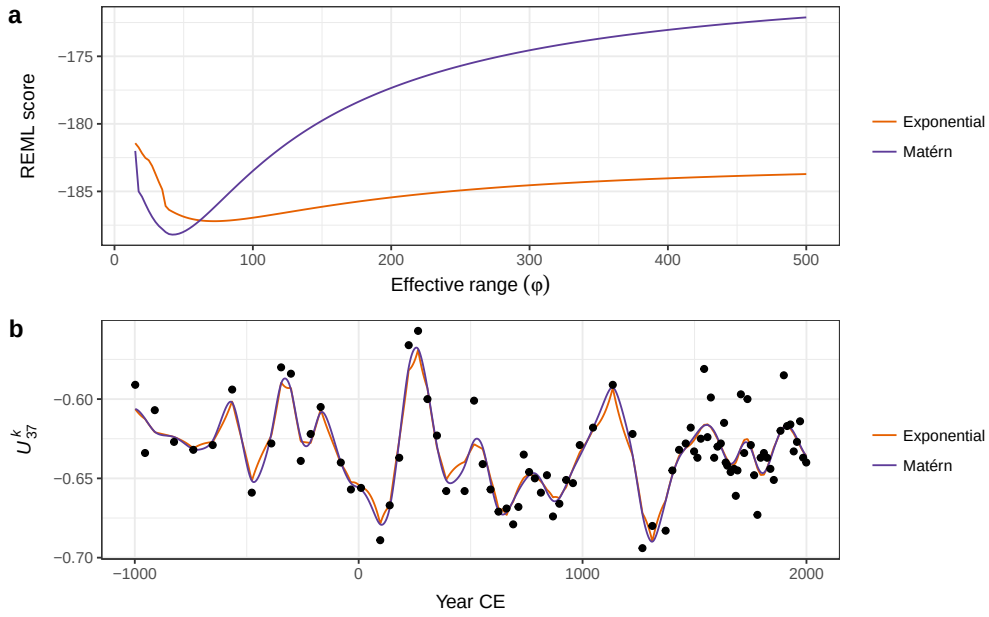
```
## Power exponential
gp3 <- gam(UK37 ~ s(Year, k = 45, bs = "gp", m = c(2, effRange3, 1)),
           data = braya,
           method = "REML", weights = sampleInterval / mean(sampleInterval))

newd <- with(braya, data.frame(Year = seq(min(Year), max(Year),
                               length.out = 1000)))
p.gp2 <- transform(newd,
                   fitted = predict(gp2, newdata = newd, type = "response"),
                   effRange = round(effRange2))
p.gp3 <- transform(newd,
                   fitted = predict(gp3, newdata = newd, type = "response"),
                   effRange = round(effRange3))
## pred <- rbind(p.gp1, p.gp2, p.gp3)
pred <- rbind(p.gp2, p.gp3)
pred <- transform(pred, effRange = factor(effRange),
                  cor = rep(c("Matérn", "Exponential"), each = nrow(newd)))
```

152 The estimated trends are plotted using

```
## plot at two values of h
gp.plt2 <- ggplot(pred, aes(x = Year, y = fitted, colour = cor)) +
    geom_line() + theme(legend.position = "right") +
    geom_point(aes(x = Year, y = UK37), data = braya, inherit.aes = FALSE) +
    scale_colour_manual(name = "", values = c("#e66101","#5e3c99")) +
    labs(y = braya_ylabel, x = "Year CE")
```

153 whilst Figure 12 in the manuscript was prepared using

```
plot_grid(proflik.plt, gp.plt2, ncol = 1, labels = c("a","b"),
          align = "hv", axis = "lr")
```



7 Adaptive smooths

The adaptive smooth was fitted to the Braya-Sø data by adding `bs = "ad"` to the `s()` term in the model formula. The other aspects of the fit are as previously used for the other models, REML smoothness selection and observational weights:

```
## Adaptive spline, weights as sampleInterval
mod_ad <- gam(UK37 ~ s(Year, k = 45, bs = "ad"), data = braya,
              method = "REML",
              weights = sampleInterval / mean(sampleInterval))
```

8 Compare various trends

For the model comparison, I refitted all the models for consistency; the code to fit each of the

1. Thin plate regression spline,
2. Gaussian process spline (Matérn correlation functions), and
3. Adaptive smoother

is shown below.

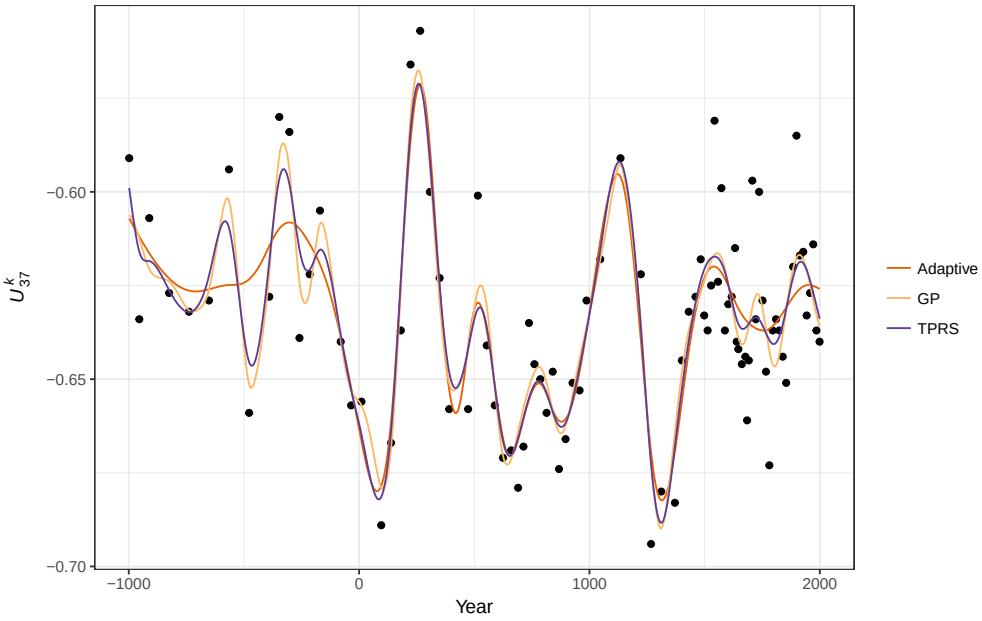
```
## model it using gam()
effRange <- effRange2

## TPRS, weights as sampleInterval, k = needs to be higher
mod_tprs <- gam(UK37 ~ s(Year, k = 45, bs = "tp"), data = braya,
```

```
                method = "REML",
                weights = sampleInterval / mean(sampleInterval))

## Gaussian process, Matern, kappa = 1.5, weights as sampleInterval
mod_gp <- gam(UK37 ~ s(Year, k = 45, bs = "gp", m = c(3, effRange)),
              data = braya,
              method = "REML",
              weights = sampleInterval / mean(sampleInterval))

## Adaptive spline, weights as sampleInterval
mod_ad <- gam(UK37 ~ s(Year, k = 45, bs = "ad"), data = braya,
              method = "REML",
              weights = sampleInterval / mean(sampleInterval))
```

We write a small function to predict from each model over the range of Year and return the data in tidy format for plotting. The plot produce reproduces figure 13 in the manuscript.

```
## wrap this in a function that will return all the plots & derived objects
processGAM <- function(mod) {
    ## Predict from model
    N <- 500
    newYear <- with(braya,
                    data.frame(Year = seq(min(Year), max(Year),
                                          length.out = N)))
    newYear <- cbind(newYear,
                     data.frame(predict(mod, newYear, se.fit = TRUE)))

    out <- list(objects = newYear)
    out
}

plts_gp   <- processGAM(mod = mod_gp) # Gaussian process smooth with weights
plts_ad   <- processGAM(mod = mod_ad) # Adaptive smooth with weights
plts_tprs <- processGAM(mod = mod_tprs) # TPRS with weights

pltData <- do.call("rbind", lapply(list(plts_gp, plts_ad, plts_tprs),
                                   `[[`, "objects"))
pltData <- transform(pltData, Model = rep(c("GP", "Adaptive", "TPRS"),
                                each = nrow(plts_gp$objects)))

allFits <- ggplot(pltData, aes(x = Year, y = fit)) +
    geom_point(aes(x = Year, y = UK37), data = braya) +
    geom_line(aes(colour = Model)) + labs(y = braya_ylabel, x = "Year") +
    theme(legend.position = "right") +
    scale_colour_manual(name = "",
```

```
                          values = c("#e66101", "#fdb863", "#5e3c99"))
allFits
```



9 Accounting for age-model uncertainty

The manuscript proposed to simulate from the posterior distribution of the fitted age model as a way to account for age-model uncertainty. The first step in the process is to fit the age model from which to simulate new age models. This was done using the *scam* package for a *shape-constrained GAM*, with the age-model spline constrained to be monotonic decreasing (`bs = "mpd"`).

To make this section self-contained, I refitted the Small Water GAM plus CAR(1) model

```
knots <- with(small, list(Year = seq(min(Year), max(Year), length = 14)))
mod <- gamm(d15N ~ s(Year, k = 15), data = small, method = "REML",
            correlation = corCAR1(form = ~ Year),
            knots = knots)
```

and then we load the ^{210}Pb dating results for the dated core sections.

```
swAge <- read.csv("./data/small-water/small1-dating.csv")
```

before fitting the shape-constrained GAM. Currently, *scam* can only fit models using GCV smoothness selection. I used the `gamma` argument here to add a larger penalty for more-complex models. Each effective degree of freedom used by the spline is counted as 1.4 degrees of freedom in the GCV score.

```
## monotonic spline age-depth model
swAge$Error[1] <- 1.1
swAgeMod <- scam(Date ~ s(Depth, k = 5, bs = "mpd"), data = swAge,
                 weights = 1 / swAge$Error, gamma = 1.4)
```

Note that I added a small amount of error to the surface sample age as the model cannot be fitted if an observation has 0 weight.

Next, predict from the estimated age model, and draw 25 samples from the posterior distribution using `simulate()`. The results are tidied into a format suitable for further processing and plotting. Note that the posterior samples here are only used for plotting.

```
## predict from the age model for a smooth set of points in `Depth`
newAge <- with(swAge, data.frame(Depth = seq(min(Depth), max(Depth),
                                             length.out = 200)))
newAge <- transform(newAge,
                    fitted = predict(swAgeMod, newdata = newAge,
                                     type = "response"))
newSims <- as.data.frame(simulate(swAgeMod, nsim = 25, newdata = newAge))
newSims <- cbind(Depth = newAge$Depth, newSims)
newSims <- gather(newSims, Simulation, Age, -Depth)
```

In the next code chunk, I draw 100 samples from the posterior distribution of the age model, but notice that I pass in the `small` data to `newdata` in the call to `simulate()` as the locations I want new age estimates for are the depths for which we have δ^{15}N values. A small function (`fitSWModels`) is written to prepare each simulation for fitting and then actually fit the GAM plus CAR(1) model using the updated age information.

```
## simulate from age model; each column is a simulation
ageSims <- simulate(swAgeMod, nsim = 100, newdata = small, seed = 42)
ageSims <- as.data.frame(ageSims)

fitSWModels <- function(x, y, knots) {
    dat <- data.frame(d15N = y, Year = x)
    m <- gamm(d15N ~ s(Year, k = 15), data = dat, method = "REML",
              correlation = corCAR1(form = ~ Year), knots = knots)
}

## generate new trends using draws from age-model posterior
simTrendMods <- lapply(ageSims, fitSWModels, y = small$d15N, knots = knots)


## function wrapper to predict new trends at locations over the
## range of `Year`
predSWModels <- function(mod, newdata) {
    predict(mod$gam, newdata = newdata, type = "response")
```

```
}

## predict from fitted model to produce a smooth trend for each posterior
## sample
simTrends <- lapply(simTrendMods, predSWModels, newdata = newYear)

## arrange in a tidy format form plottings
simTrends <- data.frame(Year  = with(newYear, rep(Year, length(simTrends))),
                        Trend = unlist(simTrends),
                        Group = rep(seq_along(simTrends),
                                    times = lengths(simTrends)))
```

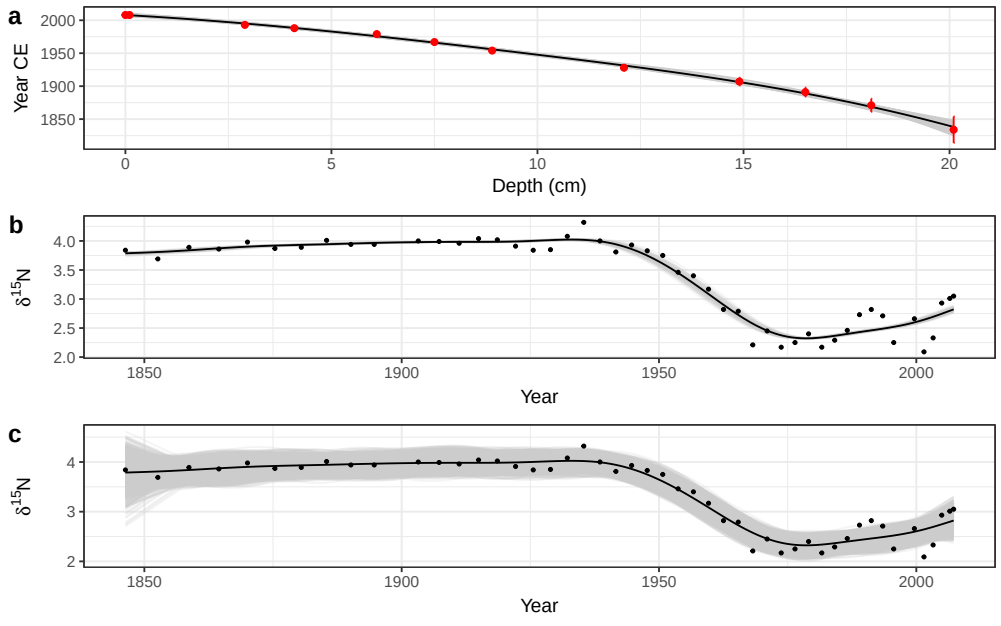
The next chunk does the final step in the process. For each of the models we just fitted to include age model uncertainty, we simulate 50 draws from the model posterior distribution. We start with a wrapper function around the `simulate()` code we want to run on each model, then do the actual posterior draws for each model using `lapply()`. The final step just arranges data for plotting.

```
## wrapper to simulate from a fitted GAM with the arguments/settings
## I want
simulateSWModels <- function(mod, newdata, nsim, seed = 42) {
    sims <- simulate(mod, nsim = nsim, newdata = newdata, seed = seed)
    as.vector(sims)
}

## now do the posterior simulation
NSIM <- 50     # number of posterior samples *per* model
simSimulate <- lapply(simTrendMods, simulateSWModels, newdata = newYear,
                      nsim = NSIM, seed = 42)

## arrange in a tidy format
simSimulate <-
  data.frame(Year  = with(newYear,
                          rep(Year, times = NSIM * length(simSimulate))),
             Trend = unlist(simSimulate),
             Group = rep(seq_len(NSIM * length(simSimulate)),
                         each = nrow(newYear)))
```

Each of the steps is visualized using the plot code shown below.

```
plt1 <- ggplot(swAge, aes(y = Date, x = Depth)) +
    geom_line(data = newSims,
              mapping = aes(y = Age, x = Depth, group = Simulation),
              alpha = 1, colour = "grey80") +
    geom_line(data = newAge, mapping = aes(y = fitted, x = Depth)) +
    geom_point(size = 1.5, colour = "red") +
```

```
    geom_errorbar(aes(ymin = Date - Error, ymax = Date + Error, width = 0),
                  colour = "red") +
    labs(y = "Year CE", x = "Depth (cm)")

plt2 <- ggplot(simTrends, aes(x = Year, y = Trend, group = Group)) +
    geom_line(alpha = 0.1, colour = "grey80") +
    geom_line(data = newYear,
              mapping = aes(x = Year, y = fit), inherit.aes = FALSE) +
    geom_point(data = small,
               mapping = aes(x = Year, y = d15N),
               inherit.aes = FALSE, size = 0.7) +
    labs(x = "Year", y = d15n_label)

plt3 <- ggplot(simSimulate, aes(x = Year, y = Trend, group = Group)) +
    geom_line(alpha = 0.2, colour = "grey80") +
    geom_point(data = small,
               mapping = aes(x = Year, y = d15N),
               inherit.aes = FALSE,
               size = 0.7) +
    geom_line(data = newYear,
              mapping = aes(x = Year, y = fit),
              inherit.aes = FALSE) +
    labs(x = "Year", y = d15n_label)

plot_grid(plt1, plt2, plt3, ncol = 1, labels = "auto", align = "hv",
          axis = "lrtb", rel_widths = c(0.5, 1, 1))
```



This reproduces figure 14 from the manuscript.

10 Session information

```
devtools::session_info()
```

```
#> Session info -------------------------------------------------------------
#>  setting  value
#>  version  R version 3.4.4 Patched (2018-03-17 r74422)
#>  system   x86_64, linux-gnu
#>  ui       X11
#>  language (EN)
#>  collate  en_CA.UTF-8
#>  tz       America/Regina
#>  date     2018-05-14
#> Packages -----------------------------------------------------------------
#>  package    * version date       source
#>  backports    1.1.2   2017-12-13 CRAN (R 3.4.3)
#>  base       * 3.4.4   2018-03-18 local
#>  codetools    0.2-15  2016-10-05 CRAN (R 3.4.4)
#>  colorspace   1.3-2   2016-12-14 CRAN (R 3.4.1)
#>  compiler     3.4.4   2018-03-18 local
#>  cowplot    * 0.9.2   2017-12-17 CRAN (R 3.4.3)
#>  datasets   * 3.4.4   2018-03-18 local
#>  devtools     1.13.5  2018-02-18 CRAN (R 3.4.4)
#>  digest       0.6.15  2018-01-28 CRAN (R 3.4.4)
#>  evaluate     0.10.1  2017-06-24 CRAN (R 3.4.1)
#>  ggplot2    * 2.2.1   2016-12-30 CRAN (R 3.4.1)
#>  glue         1.2.0   2017-10-29 CRAN (R 3.4.2)
#>  graphics   * 3.4.4   2018-03-18 local
#>  grDevices  * 3.4.4   2018-03-18 local
#>  grid         3.4.4   2018-03-18 local
#>  gtable       0.2.0   2016-02-26 CRAN (R 3.4.1)
#>  htmltools    0.3.6   2017-04-28 CRAN (R 3.4.1)
#>  knitr        1.20    2018-02-20 CRAN (R 3.4.4)
#>  labeling     0.3     2014-08-23 CRAN (R 3.4.1)
#>  lattice      0.20-35 2017-03-25 CRAN (R 3.4.4)
#>  lazyeval     0.2.1   2017-10-29 CRAN (R 3.4.2)
#>  magrittr     1.5     2014-11-22 CRAN (R 3.4.1)
#>  MASS         7.3-49  2018-02-23 CRAN (R 3.4.4)
#>  Matrix       1.2-14  2018-04-09 CRAN (R 3.4.4)
#>  memoise      1.1.0   2017-04-21 CRAN (R 3.4.1)
#>  methods      3.4.4   2018-03-18 local
#>  mgcv       * 1.8-23  2018-01-21 CRAN (R 3.4.4)
#>  munsell      0.4.3   2016-02-13 CRAN (R 3.4.1)
```

```
#>  nlme       * 3.1-137 2018-04-07 CRAN (R 3.4.4)
#>  pillar       1.2.1   2018-02-27 CRAN (R 3.4.4)
#>  plyr         1.8.4   2016-06-08 CRAN (R 3.4.1)
#>  purrr        0.2.4   2017-10-18 CRAN (R 3.4.2)
#>  Rcpp         0.12.16 2018-03-13 CRAN (R 3.4.4)
#>  rlang        0.2.0   2018-02-20 CRAN (R 3.4.4)
#>  rmarkdown  * 1.9     2018-03-01 CRAN (R 3.4.4)
#>  rprojroot    1.3-2   2018-01-03 CRAN (R 3.4.3)
#>  scales       0.5.0   2017-08-24 CRAN (R 3.4.1)
#>  scam       * 1.2-2   2017-09-24 CRAN (R 3.4.3)
#>  schoenberg * 0.0-6   2018-04-12 Github (gavinsimpson/schoenberg@f9b8a84)
#>  splines      3.4.4   2018-03-18 local
#>  stats      * 3.4.4   2018-03-18 local
#>  stringi      1.1.7   2018-03-12 CRAN (R 3.4.4)
#>  stringr      1.3.0   2018-02-19 CRAN (R 3.4.4)
#>  tibble       1.4.2   2018-01-22 CRAN (R 3.4.3)
#>  tidyr      * 0.8.0   2018-01-29 CRAN (R 3.4.4)
#>  tools        3.4.4   2018-03-18 local
#>  utils      * 3.4.4   2018-03-18 local
#>  withr        2.1.2   2018-03-15 CRAN (R 3.4.4)
#>  yaml         2.1.18  2018-03-08 CRAN (R 3.4.4)
```