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TECHNICAL NOTE

Dendroclimatic calibration in *R*: The *bootRes* package for response and correlation function analysis

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ABSTRACT

To understand the effect of climate on tree-ring features, such as width or density, tree-ring data have to be calibrated against instrumental records. The high degree of multicollinearity among monthly time series of climate data violates the assumption of independent predictor variables in ordinary least squares regression. Bootstrapped confidence intervals of parameter estimates via regression against the principle components of the predictor variables are a possible solution to that problem. Package *bootRes* for *R* implements a flexible interface for bootstrapped response and correlation function analysis and tackles some shortcomings of currently available software. Given the increasing popularity of the free *R* software for statistical analysis, *bootRes* should facilitate both using *R* as a computational environment among tree-ring scientists and implementing new approaches to dendroclimatic calibration.

Introduction

The properties of tree-rings (such as width or density) are often regressed against instrumental data at monthly resolution to understand the particular climate variables to which these properties are sensitive. A general problem of these calibration approaches is the pronounced intercorrelation of the climatic variables used as predictors (Cropper, 1984), a phenomenon also known as multicollinearity. The linear regression model $\boldsymbol{y} = \boldsymbol{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$ is based on the condition that the predictor variables are independent of one another. Using predictors with a high amount of multicollinearity violates this assumption and leads to imprecise and unstable estimates $\boldsymbol{b} = (\boldsymbol{X}^{\top}\boldsymbol{X})^{-1}\boldsymbol{X}^{\top}\boldsymbol{y}$ of regression coefficients and their statistical significance, the latter possibly leading to over- or under-fitted models (Fritts, 1976).

An alternative to multivariate linear or stepwise linear regression in paleoclimatic calibration (with a focus on tree-ring data) was presented by Fritts et al. (1971) in the form of *response function analysis*, where the predictand is regressed against the principal components of the predictor variables. This technique has the drawback that classical measures of significance produce incorrect confidence intervals for the regression coefficients (Guiot, 1991; Morzuch and Ruark, 1991), eventually producing over-fitted response functions. As a solution, Guiot (1991) proposed bootstrapping (Efron and Tibshirani, 1986) to obtain more accurate results for response functions, then Biondi (1997) introduced the concept of applying bootstrapped correlation and response functions to multiple time intervals for assessing the stationarity of such responses. This approach, as shown in detail by Biondi (2000), provided a numerical way to both define and investigate what later became known as the "divergence problem" (D'Arrigo et al., 2008). In the field of tree-ring science, bootstrapped response functions are becoming increasingly popular, as shown by the increasing number of citations over time for software that implements them (Fig. 1). Typical application areas include assessing spatial (e.g., Mérian et al., 2011; Zang et al., 2011b; Lloyd et al., 2011), temporal (e.g., Mérian et al., 2011; Filippo et al., 2010) and ontogenetic (e.g., Zang et al., 2011a; Mérian and Lebourgeois, 2011) patterns of the climate sensitivity of tree growth, and the reconstruction of environmental factors from tree-ring records (e.g., Duncan et al., 2010; Hart et al., 2010).

The package *bootRes* for *R* (R Development Core Team, 2012) presented in this paper is an attempt to overcome the shortcomings of existing software packages, such as being bound to specific operating systems, or not providing interfaces or scripting hooks for batch processing large amounts of data. Our objective is to provide a unified interface for calibration of tree-ring and other proxy data against multiple instrumental time series. The

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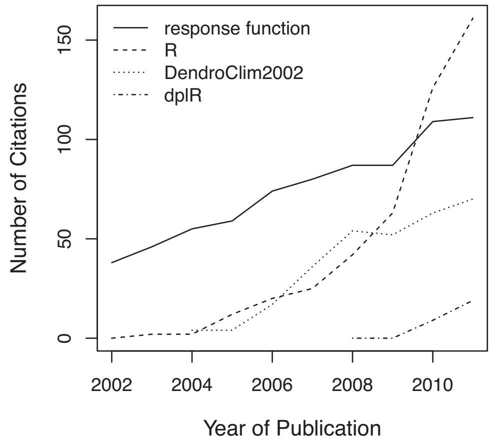

Fig. 1. Publications in tree-ring sciences that contain references to *R*, DendroClim2002 and dplR. Boolean search operations were used with Google Scholar (http://scholar.google.com) to find the number of publications (search terms were TREE-RING* OR DENDROCHRONOLOGY OR DENDROECOLOGY) that reference (logical AND) response functions (search term "RESPONSE FUNCTION*"), the *R* software package (search term "R DEVELOPMENT CORE TEAM"), DendroClim2002 (search term "DENDROCLIM2002"), or dplR ("DPLR").

functionality of *bootRes* is modelled closely after *DENDROCLIM2002* (Biondi and Waikul, 2004), a very popular package for dendroclimatic calibration (Fig. 1). Contrary to the platform-dependent *DENDROCLIM2002*, we use *R* as the base for the implementation. This is based on the rationale that *R* is becoming an increasingly popular choice as the primary analytic environment among researchers across disciplines (for a bibliometric overview, see Firth, 2011), including dendrochronology (Fig. 1).

bootRes is designed to interface with package *dplR* (Bunn et al., 2012), i.e., tree-ring chronologies produced with *dplR* can directly be used with *bootRes*. The latest stable version of *bootRes* is available from the Comprehensive *R* Archive Network at http://CRAN.R-project.org/package=bootRes. The code is maintained as a *Git* repository on *Github* (http://github.com/znag/bootRes), where users can also file issues and claim pull requests for changes to the code.

Numerical analysis

Generally, the approach used in response (and correlation) function analysis is an indirect regression (Christiansen, 2011), i.e., the proxies are modelled as a function of the climatic variables. Let $\boldsymbol{y}$ be a $n \times 1$ vector of a univariate response variable (some tree-ring property), and $\boldsymbol{X}$ the $n \times k$ matrix of standardized predictor variables. In dendroclimatic calibration, $\boldsymbol{X}$ usually consists of monthly temperature and precipitation data affected by varying amounts of multicollinearity (Cropper, 1984). Because of multicollinearity in $\boldsymbol{X}$ the use of ordinary least squares (OLS) to estimate the $k \times 1$ vector $\boldsymbol{b}$ of parameters of the model

$$\boldsymbol{y} = \boldsymbol{Xb} + \boldsymbol{\epsilon}$$

yields unstable results, as the elements of the OLS estimate of $\boldsymbol{b}(\hat{\boldsymbol{b}})$ may have inflated variances. To overcome that shortcoming, the original variables $\boldsymbol{X}$ are orthogonalized so that

$$\boldsymbol{y} = \boldsymbol{XVV}^{\top}\boldsymbol{b} + \boldsymbol{\epsilon} = \boldsymbol{Za} + \boldsymbol{\epsilon} \qquad (1)$$

with $\boldsymbol{V}$ being the $k \times k$ matrix of normalized eigenvectors of $\boldsymbol{X}$, $\boldsymbol{Z}$ being the $n \times k$ matrix of principal components $\boldsymbol{XV}$ of $\boldsymbol{X}$, and the $k \times 1$ vector $\boldsymbol{a} = \boldsymbol{V}'\boldsymbol{b}$ being the linear transformation of the original regression coefficients $\boldsymbol{b}$. For the final estimation, $\boldsymbol{a}$ can be transformed back to the original parameter space because $\boldsymbol{V}$ is an orthogonal matrix and thus $\boldsymbol{b} = \boldsymbol{Va}$.

Usually, the method further involves partitioning $\boldsymbol{V}$ into $[\boldsymbol{V_1} \vdots \boldsymbol{V_2}]$ where $\boldsymbol{V_1}$ is a $k \times r$ matrix of important eigenvectors (high eigenvalues) and $\boldsymbol{V_2}$ a $k \times s$ matrix of eigenvectors that are deemed unimportant because of low eigenvalues (Morzuch & Ruark, 1991). This step ensures that the resulting matrix is farther from being singular, thus further reducing the amount of multicollinearity. Eq. (1) can be rewritten as

$$\boldsymbol{y} = \boldsymbol{X}[\boldsymbol{V}_1 \vdots \boldsymbol{V}_2]\boldsymbol{a} + \boldsymbol{\epsilon}, \qquad (2)$$

and $\boldsymbol{a}$ can correspondingly be written as $[\boldsymbol{a}_1 \vdots \boldsymbol{a}_2]'$, where $\boldsymbol{a}_1$ is a $r \times 1$ vector associated with $\boldsymbol{V}_1$, and $\boldsymbol{a}_1$ a $s \times 1$ vector associated with $\boldsymbol{V}_2$, so that

$$\boldsymbol{y} = \boldsymbol{XV}_1\boldsymbol{a}_1 + \boldsymbol{XV}_2\boldsymbol{a}_2 + \boldsymbol{\epsilon} = \boldsymbol{Z}_1\boldsymbol{a}_1 + \boldsymbol{Z}_2\boldsymbol{a}_2 + \boldsymbol{\epsilon}. \qquad (3)$$

There has been some discussion in the literature about how many eigenvectors to retain; for an overview see Fritts (1991). In its current implementation, *bootRes* uses the PVP criterion (Guiot, 1990), i.e., eigenvectors are sorted according to descending eigenvalues and r is then the number of eigenvectors whose associated eigenvalues have a cumulative product greater than 1.

The estimators of the response function are obtained by application of ordinary least squares on a modified model that has been simplified by taking out the unimportant components $\boldsymbol{Z}_2$ so that

$$\boldsymbol{y} = \boldsymbol{Z}_1\boldsymbol{a}_1 + \boldsymbol{\epsilon}^*. \qquad (4)$$

with $\boldsymbol{\epsilon}^* = \boldsymbol{Z_2a_2} + \boldsymbol{\epsilon}$. The $r \times 1$ vector $\boldsymbol{a}_1$ is padded with $s - r$ zeros to obtain a $k \times 1$ vector $\boldsymbol{a}_1^*$. This vector can be used to obtain an estimator of $\boldsymbol{b}$ by translation back to the original parameter space via $\boldsymbol{Va}_1^* = \boldsymbol{b}^*$. Therefore, $\boldsymbol{b}^*$ is a $k \times 1$ vector, indicating that all of the original variables have been retained.

bootRes uses bootstrap resampling (Efron and Tibshirani, 1986) to calculate response coefficients on 1000 samples drawn at random with replacement from the calibration set. Median coefficients are judged significant at the $P = 0.05$ level when their absolute values exceed half the difference between the 97.5th quantile and the 2.5th quantile (Biondi and Waikul, 2004).

Correlation function analysis uses Pearson sample correlation estimates computed between the tree-ring parameter and each of the climatic predictors. Bootstrap resampling is used to obtain robust estimates of the significance of correlation function coefficients using the percentile range method described above.

Package *bootRes* in practice

Static response functions

The package is loaded into *R* using the `library()` or `require()` command:

```
R> library("bootRes")
```

The package *dplR* is recommended but not necessarily needed.

Purely as an example, we use a data set consisting of tree-ring widths from 10 spruce trees growing near Munich, Germany, and the corresponding climatic data in monthly resolution (Zang et al., 2011a). The individual raw tree-ring width series (2 cores per tree) have been subject to detrending using cubic splines with 50% frequency cutoff of 60 years (Cook and Peters, 1981), and are averaged using Tukey's biweight robust mean (Mosteller and Tukey, 1977). *bootRes* uses the same data model for chronologies like *dplR*, namely a `data.frame` with the values in one column and the corresponding years as `rownames`.

Function `read.crn` of package *dplR* provides an easy way of getting chronology data in standard decadal file format (see http://www.ncdc.noaa.gov/paleo/treeinfo.html for a detailed description of the decadal format) into an *R* session. Note that shortened console output is indicated by horizontal dots.

```
R> data("muc.spruce")
R> muc.spruce
        mucstd samp.depth
1939 0.4054986          1
1940 0.3146843          1
1941 0.6424530          1
1942 0.7963554          1
1943 1.3833328          3
1944 1.6567071          3
...
```

For the formatting of climatic data, three options exist: climatic data can either consist of at least 3 columns, where the first column signifies year, the second column month and every further column holds a climatic parameter. The names of the columns are not important, but one may want to choose meaningful names for the climatic variables, as their names will be recycled by different functions of *bootRes*. Note, that only complete years (months 1–12) may be provided. An example of this formatting convention is provided with example data `muc.clim` in *bootRes*:

```
R> data("muc.clim")
R> muc.clim
  year   month temp   prec
1 1949   1     -0.4   44.9
2 1949   2     -0.7   19.2
3 1949   3      1.3   33.9
4 1949   4      9.8   58.9
5 1949   5     11.1  250.5
6 1949   6     13.1   70.7
...
```

Furthermore, climatic data can consist of `data.frames` with 13 columns, representing year and 12 monthly observations for one parameter. This formatting corresponds to the input files used for *DENDROCLIM2002* (Biondi and Waikul, 2004). An illustration of the formatting is given by example data `rt.temp` and `rt.prec` in *bootRes*.

```
R> data("rt.temp")
R> rt.temp
  Year  Jan  Feb Mar  Apr  May  Jun  Jul  Aug  Sep  Oct Nov  Dec
1 1948  2.9  0.4 6.2  9.7 14.0 15.6 15.6 16.2 13.2  8.4 3.4 -0.9
2 1949  0.2  0.3 2.1 10.7 11.8 14.2 18.6 17.5 16.8 10.6 3.0  2.2
3 1950 -1.4  2.7 4.6  6.4 13.8 17.9 18.8 17.4 12.4  7.5 4.0 -2.9
4 1951  1.6  1.9 2.4  7.4 11.8 14.8 17.5 17.1 14.2  7.5 5.5  0.8
...
```

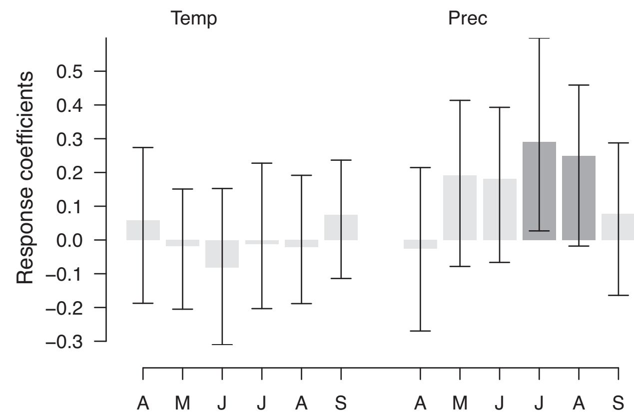

Fig. 2. Response coefficients for temperature and precipitation from April to September for a tree-ring chronology from a sandy and dry site near Rothenburg ob der Tauber, Northern Bavaria, Germany. The darker bars indicate a coefficient significant at $P < 0.05$, the lines represent the 95%-confidence interval.

Either a single one of these `data.frames` can be provided, or a list consisting of an arbitrary number of similarly formatted `data.frames`.

The bootstrapped response function is now calculated by invoking function `dcc()`.

```
R> my.calib <- dcc(muc.spruce, muc.clim)
|==================================================| 100%
time span considered: 1949 - 2007
```

By default `dcc` will determine the longest shared time period of tree-ring and climatic data and will calculate the response function for that time span. If a subset of the data is to be used as calibration set, the parameter `timespan` can be set accordingly. The months to be used for calibration can be set by `start` and `end`; these settings default to −6 (previous June) and 9 (current September) respectively. These 16 months correspond to a total of 32 predictors if two climatic variables (such as precipitation and temperature) are used. Because of the potential large number of predictors, *bootRes* will issue an error message if the period of overlap between the tree-ring chronology and the instrumental records is less than the number of predictors. It is also strongly recommended that investigators carefully consider the appropriateness of default values for the first and last month of the calibration window, since growing seasons can vary with species and regions, and the use of prewhitened chronologies would not be consistent with a window longer than 12 months. A status bar informs about the progress of the bootstrap resampling, but one may suppress this (e.g., for use with *SWeave*, Leisch, 2002) by setting parameter `sb = F`.

The names of climatic variables are recycled from the `colnames` of the climatic data. If other variable names shall be used these can be provided using the `vnames` parameter. The new variable names consist of the recycled or provided variable names suffixed with the year (previous or current) and month.

The result of `dcc` is a `data.frame` containing the parameter values, significance flags and upper and lower 95% confidence intervals.

```
R> my.calib
                     coef significant    ci.lower   ci.upper
temp.prev.jun -0.087715239       FALSE -0.29440033 0.11648780
temp.prev.jul -0.023778738       FALSE -0.22355529 0.16933096
temp.prev.aug -0.117458801       FALSE -0.35465337 0.07772130
...
temp.curr.jan -0.066040846       FALSE -0.27334815 0.14312929
temp.curr.feb  0.152557889       FALSE -0.07365590 0.35969768
temp.curr.mar  0.026412244       FALSE -0.18119799 0.28976224
...
prec.prev.jun  0.020113217       FALSE -0.21849622 0.21761482
prec.prev.jul -0.041048340       FALSE -0.24249233 0.15147634
prec.prev.aug -0.024640444       FALSE -0.25337174 0.20690825
...
prec.curr.jan  0.087499926       FALSE -0.13015981 0.29478896
prec.curr.feb  0.101294207       FALSE -0.06932484 0.28887250
prec.curr.mar  0.017735144       FALSE -0.24395644 0.29452197
...
```

In the above example, none of the climatic parameters was judged significant at the $P < 0.05$ level. This is typical for a forest site not strongly limited by climate: the forest stand in which the trees were sampled is characterized by ample precipitation amounts throughout the year.

To use *bootRes* with *DENDROCLIM2002*-formatted climatic data, use

```
R> data("rt.spruce")
R> data("rt.temp")
R> data("rt.prec")
R> my.calib2 <- dcc(rt.spruce, list(rt.temp, rt.prec), vnames =
c("temp", "prec"), start = 4, end = 9)
```

This data set is a spruce chronology from a sandy and dry site with periodic phases of drought during the summer months in Rothenburg, located approximately 200 km in north-western direction from the first stand (Zang et al., 2011a). Like for the first data set, 20 cores from 10 trees were subject to spline detrending (50% frequency cutoff for 60 year period), and then averaged to a chronology using Tukey's biweight robust mean. This time, only the growth period of the current year (April-September) is used for calibration, and climatic limitation of tree-growth is reflected by the response parameters:

```
R> my.calib2
                     coef significant    ci.lower  ci.upper
temp.curr.apr  0.05905965       FALSE -0.18753599 0.2739435
temp.curr.may -0.01873640       FALSE -0.20504353 0.1509720
temp.curr.jun -0.08135238       FALSE -0.31051350 0.1524699
temp.curr.jul -0.01181418       FALSE -0.20339449 0.2275644
temp.curr.aug -0.02080866       FALSE -0.18852915 0.1916090
temp.curr.sep  0.07427579       FALSE -0.11409067 0.2365764
prec.curr.apr -0.02598193       FALSE -0.26971961 0.2145323
prec.curr.may  0.19181285       FALSE -0.07842066 0.4136406
prec.curr.jun  0.18085982       FALSE -0.06644810 0.3929813
prec.curr.jul  0.29069076        TRUE  0.02689140 0.5984969
prec.curr.aug  0.24896661        TRUE -0.01807863 0.4589387
prec.curr.sep  0.07765448       FALSE -0.16404284 0.2876011
```

Obviously, moisture variability in July and August has a significant controlling influence on tree growth. To visualize the results, the set of response coefficients can be plotted (Fig. 2):

```
R> dcplot(my.calib2)
```

The results from *bootRes* are numerically equivalent to the results from *DENDROCLIM2002*, given the variability introduced by the bootstrap method (Fig. 3). Also, the same set of parameters are judged significant in both implementations.

Moving response functions

For reconstruction purposes it is generally assumed that proxy data obey the principle of uniformity – for tree-rings this means that the physical and biological processes that are currently linked with patterns of tree growth have been operating similarly ("uniformly") in the past (Fritts, 1976). While this principle remains valid today, it should not be confused with the issues of non-stationarity and non-linearities in dendroclimatic relationships. A possible example are climate-signal-age effects, that arise when xylem layers close to the pith (hence with a younger biological age) contain different climatic information compared to more recent, "adult" rings (Esper et al., 2008). Although it is crucial to assess the temporal stability of dendroclimatic relationships, one should not forget that, without rigorous field experiments, we cannot know if a change in signals is due to tree age (whose effect should have been removed by the standardization method), by changing quality of the climate data (always possible given the limited lifespan of instruments and station locations), or by actual changes in the climate–tree growth relationships.

To investigate the stability of growth/climate relationships, moving response (or correlation) functions can be used. *bootRes* provides a flexible interface for moving response and correlation functions; the underlying principle is that the period of overlap between the tree-ring chronology and the instrumental time series is split into equal time periods (length and distance from each other can be chosen), for each of which a complete calibration is calculated. The size of the moving window defaults to 25 years, and *bootRes* issues an error message when this baseline length is shorter than the number of predictors.

```
R> mov.calib <- mdcc(rt.spruce, list(rt.temp, rt.prec), vnames =
c("temp", "prec"), start = 4, end = 9)
```

The interface of the moving function `mdcc()` is quite similar to `dcc()`, and so is the output, which this time is sliced into the different time periods for which independent calibrations were performed:

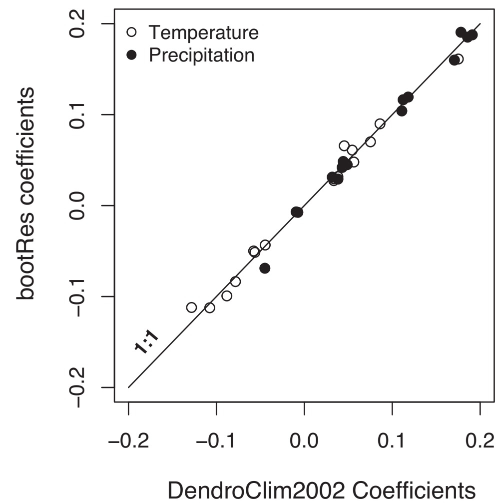

Fig. 3. Direct comparison of response coefficients for temperature and precipitation from previous June to current September for the Rothenburg spruce chronology obtained by *bootRes* and *DendroClim2002*. The correlation between both sets of parameter estimations is 0.996.

The results can be visualized with function `mdcplot()` (Fig. 4):

```
R> mdcplot(mov.calib)
```

Obviously, growth/climate relations are not stable over time, especially the positive influence of August precipitation on tree growth has gotten weaker over time, whereas the negative influence of June temperature has become stronger.

Again, the results are identical to the results obtained with *DendroClim2002* using the same data sets and settings. The correlation between the parameters estimated with both implementations range from 0.9976 to 0.9997 for the 34 individual windows.

```
R> mov.calib

               1950-1974   1951-1975    1952-1976    1953-1977 ...

temp.curr.apr  0.185468619  0.16798936  0.162005935  0.146702115 ...
temp.curr.may -0.099028582 -0.09870666 -0.145936894 -0.213266063 ...
temp.curr.jun  0.052582533  0.04948240 -0.008572624 -0.086064363 ...
temp.curr.jul -0.042932989 -0.04622819 -0.104440382 -0.092958202 ...
temp.curr.aug -0.030132061 -0.05546489 -0.008999988  0.009633602 ...
temp.curr.sep  0.067538152  0.03211490  0.076052938  0.057609580 ...
prec.curr.apr  0.042560046  0.06288620  0.146560295  0.167815247 ...
prec.curr.may  0.000171586 -0.05176082  0.081787057  0.093109608 ...
prec.curr.jun  0.282233219  0.25500423  0.177149921  0.171543466 ...
prec.curr.jul  0.018110438  0.02180999 -0.017391903 -0.076305663 ...
prec.curr.aug  0.384133822  0.36059234  0.463770073  0.367770668 ...
prec.curr.sep  0.117716483  0.12764475  0.057247876  0.120118064 ...
...
```

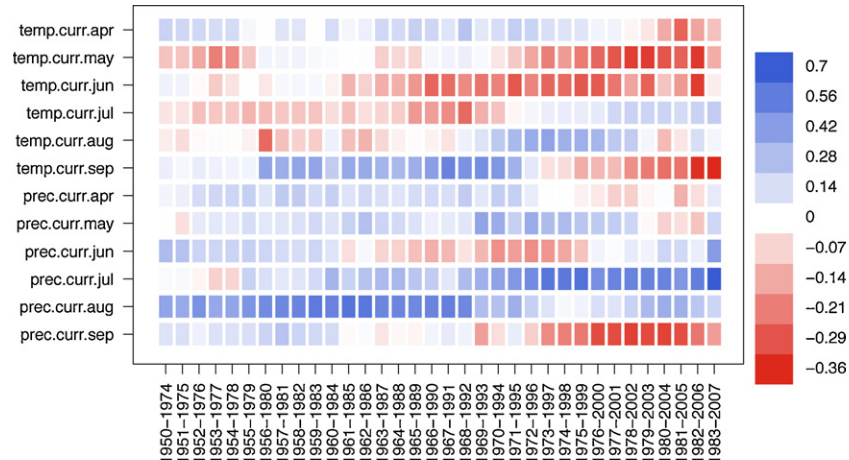

Fig. 4. Moving response functions of temperature and precipitation from April to September for a tree-ring chronology from a sandy and dry site near Rothenburg ob der Tauber, Northern Bavaria, Germany. The window size is 25 years, and the windows have been offset by one year.

Discussion

We propose the use of software package *bootRes* for climatic calibration of proxy data in *R* with a focus on tree-ring chronologies. The package is designed to be user-friendly and to interface nicely with *dplR* for chronology development and general tree-ring statistics. To that end, *bootRes* allows for different formatting options for the climatic input data, so that researchers can start to analyze their data in *R* more easily. Furthermore, default choices for model parameters are offered, but we encourage all users to treat them simply as suggestions, and to think carefully about their own research questions, available data, and geographic focus.

The package is designed in a modular fashion, so that the implementation of additional techniques is simplified. For the future, we plan on extending the package from its current state as a primarily explorative tool for data analysis towards an integrated solution for both calibration and reconstruction. We are aware of the fact that the forward modelling approach (indirect regression, Christiansen, 2011) implemented with the response and correlation functions is not directly invertible to infer climate conditional on the proxies. However, this possibility is covered within a Bayesian framework for paleoclimatic reconstruction (Tingley and Huybers, 2010; Li et al., 2010), which has yet to be fully embraced by the tree-ring science community.

Finally, we encourage others to participate in expanding the functionality of *bootRes*, either by suggesting new functions, or by actively contributing to the code base.

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