`WiSEBoot` Vignette

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1 WiSE Bootstrap Model Selection

Wild Scale-Enhanced (WiSE) Bootstrap is a variant of the wild bootstrap where the model residuals are multiplied by an additional scaling factor. Theoretical details of the general WiSE methodology may be found in (Chatterjee, 2015). This package is an implementation of the WiSE bootstrap for a specific case of the partial linear model. Namely, given an equally-spaced time series of length $T = 2^J$, $J \in \mathbb{I}^+$, we assume that the time series may be written as a partial linear model

$$Y(t) = \gamma_0 + \gamma_1 t + W\gamma + e(t) \tag{1}$$

where $Y \in \mathbb{R}^T$ is the observed data, t is a vector time indices, W is a $T-$ row matrix of a fixed wavelet basis, and γ contains the scaling and filter wavelet coefficients. Note, in many cases of the discrete wavelet transform (DWT), especially those implemented within `wavethresh`, the scaling coefficient is equivalent to γ_0. Thus, only the scaling coefficient or γ_0 should be estimated in any models where this occurs.

The quantity $W\gamma$ is a non-parametric component which may represent a signal within the data. The linear model component$(\gamma_0 + \gamma_1 t)$ would necessarily change by data application, but we claim it is adequate in the examples presented here. We propose that models of this type are useful descriptors of various time series, including climate model output. Under this partial linear model, it is of interest to estimate the set of population parameters γ_0, γ_1 and γ.

Estimating the full vector of wavelet coefficients, γ, is problematic with current methodologies. However, it is typical that the wavelet filter coefficients are sparse, containing many zero or nearly zero-valued entries. The proposed methodology takes advantage of the sparsity and chooses a strong threshold criteria for the coefficients. With data of length 2^J, filter wavelet coefficients exist for levels 0, 1, ..., $J-1$. If J_0 is our threshold, then all coefficients occuring at levels greater than J_0 are set to 0. Essentially, our models assume all fine-level filter coefficients are 0-valued in expectation. Thresholding γ in this fashion decreases the number of parameters such that consistent estimation is possible.

Assume J_0 is a set threshold level. Then, we may estimate the population parameters γ_0, γ_1 and γ consistently. Using least squares estimation, $\hat{\gamma}_0$ and $\hat{\gamma}_1$ are obtained and residuals are defined as $r(t) = Y(t) - \hat{\gamma}_0 - \hat{\gamma}_1 t$. The DWT is performed on $r(t)$ to obtain a length-T vector of wavelet coefficients. We apply the threshold and estimate γ with $\hat{\gamma}_{J_0}$. Wavelet residauls are obtained using $r_w(t) = r(t) - W\hat{\gamma}_{J_0}$.

To perform the WiSE bootstrap for model 1 with set threshold J_0, we create bootstrap series for $b = 1, 2, ..., B$

$$Y_b(t) = \hat{\gamma}_0 + \hat{\gamma}_1 t + W\hat{\gamma}_{J_0} + \tau U_b r_w(t) \tag{2}$$

where τ is a scaling parameter such that $\tau^2/T \to 0$ and $\tau \to \infty$ and the $U_i, i = 1, ..., B$ are independent, mean 0, variance 1, finite 8^{th} moment random variables. The $Y_b(t)$ are used to create bootstrap estimates $\hat{\gamma}_{0b}$, $\hat{\gamma}_{1b}$, and $\hat{\gamma}_{J_0 b}$. The wild bootstrap also allows for estimation of the error variance, which may be heteroscedastic, but this is not implemented within `WiSEBoot`. All details of these theoretical conditions and results are contained in (Chatterjee, 2015).

This WiSE bootstrap re-sampling technique is novel, as it allows for a model selection while concurrently providing (asymptotically) consistent estimators of the model parameters (Chatterjee, 2015). The prior description set the threshold level, J_0. The `WiSEBoot` package provides an automatic process to select the wavelet coefficient threshold level. For a data series of length 2^J, a WiSE bootstrap sample is created for thresholds of $J_0 \in \{0, 1, ..., J-2\}$ as well as setting all filter wavelet coefficients to 0. The selected model minimizes the mean of the mean squared-error between the bootstrap estimated model and the provided data. That is, for any J_0, we calculate the mean of the mean-squared error

$$\overline{MSE}_{J_0} = \frac{1}{TB} \sum_{b=1}^{B} < Y(t) - \hat{\gamma}_{0b} - \hat{\gamma}_{1b} t - W \hat{\gamma}_{J_0 b}, \quad Y(t) - \hat{\gamma}_{0b} - \hat{\gamma}_{1b} t - W \hat{\gamma}_{J_0 b} >$$

where $< x, y >$ is defined as the inner product of vectors x and y. The selected wavelet coefficient threshold in the model is J_0^* where

$$\overline{MSE}_{J_0^*} = \min_j \overline{MSE}_j$$

2 WiSE Bootstrap Model Selection: Simulation Example

This example uses some simulated wavelet signals to demonstrate the wavelet coefficient threshold selection. What may be considered as a population-level signal is contained in `SimulatedSmoothSeries`, which is a matrix.

```
data(SimulatedSmoothSeries)
dim(SimulatedSmoothSeries)
```

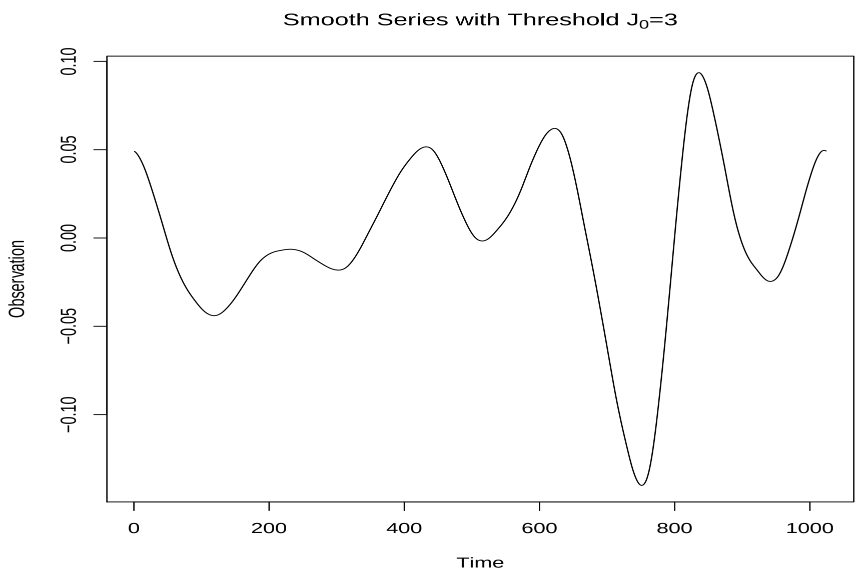
```
## [1] 1024    9
```

```
SimulatedSmoothSeries[1:3, ]
```

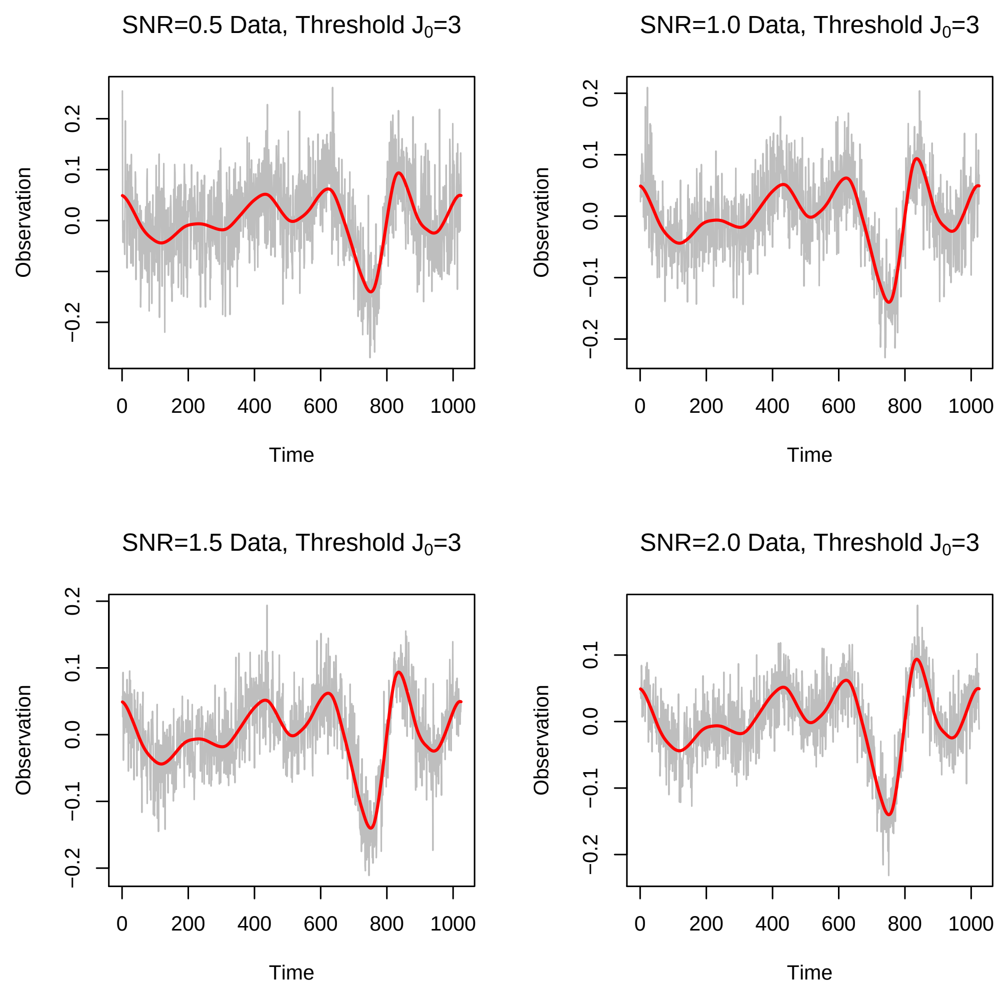
```
##              J0.0       J0.1        J0.2       J0.3        J0.4
## [1,] -0.009340405 0.01674716 0.004249168 0.04902028 -0.02750788
## [2,] -0.009343208 0.01676378 0.003836796 0.04871207 -0.02514671
## [3,] -0.009345534 0.01677582 0.003428975 0.04834426 -0.02252105
##              J0.5      J0.6      J0.7       J0.8
## [1,] -0.050660410 0.1438138 0.2153899 0.40223065
## [2,] -0.028013936 0.1572082 0.2122281 0.34668205
## [3,] -0.005142542 0.1555804 0.1611787 0.09866474
```

All signals in this matrix were generated using the `wavethresh` package with a `"DaubLeAsymm"` (Daubechies Least Asymmetric) wavelet with `8` vanishing moments and a `"periodic"` boundary condition. The column names of `SimulatedSmoothSeries` indicate the true wavelet coefficient threshold level. Let's consider the 4^{th} column. The wavelet coefficients were thresholded at the $J_0 = 3$ level. Thus, all finer-level coefficients (levels 4,5,6,7,8, and 9) were set to 0, to create this smooth signal.

Here is a plot of the signal:

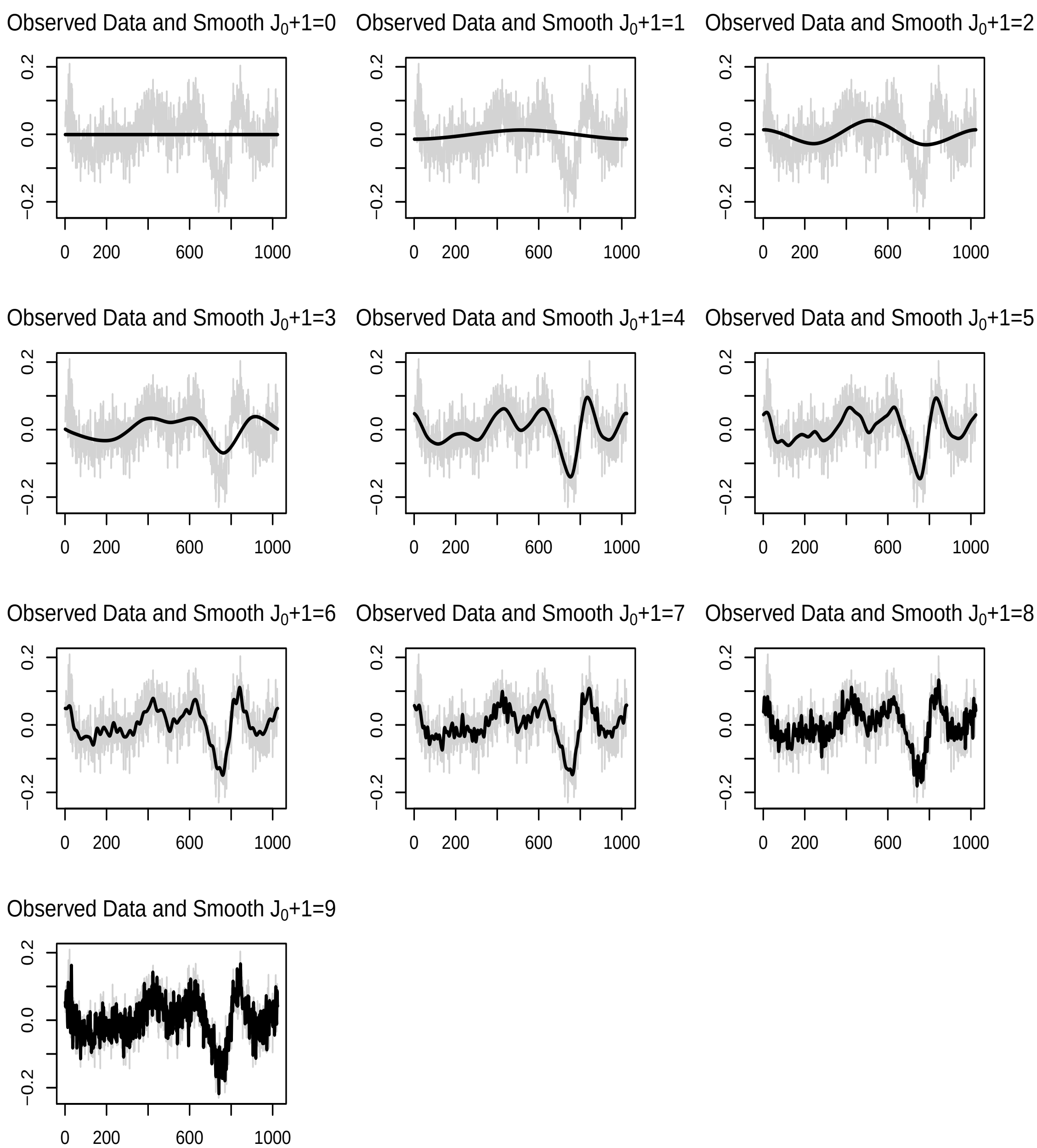


Data observed from a population signal such as this would be noisy. The matrices `SimulatedSNR0.5Series`, `SimulatedSNR1.0Series`, `SimulatedSNR1.5Series`, and `SimulatedSNR2.0Series` contain data series with population signals from `SimulatedSmoothSeries` and varying levels of added noise. Defining the signal-to-noise ratio (SNR) as (Variance of Signal)/(Variance of Noise), these matrices contain data series with SNR=0.5, 1.0, 1.5 and 2.0. It seems reasonable to assume that the signal would be more apparent in the SNR=2.0 series than the SNR=0.5 series. Here is a look at the data:



We can see that the true signal is fairly clear in each of these data series, but the lower SNR series are noisier. Typically, the analyst would not know the true signal threshold level. The `smoothTimeSeries` function allows for a quick visualization of all possible wavelet coefficient threshold levels. This is especially useful if the analyst would like to manually choose a wavelet coefficient threshold level. Using the SNR=1.0 series, we can demonstrate this capability. Note, the wavelet settings for these smooths generated below exactly match the true signals from `SimulatedSmoothSeries`. The user could change the wavelet family, filter, and boundary.

```r
smoothPlot <- smoothTimeSeries(SimulatedSNR1.0Series[ ,4], plot="all")
```



Without knowing the truth, an analyst may guess that the wavelet threshold level could be any of $J_0 \in \{2, 3, 4\}$. We can use the `WiSEBoot` function to remove the guess-work and automatically choose a wavelet threshold. As discussed in Section 1, the model which achieves the minimum of the mean-squared error is selected. Let's leave the default wavelet settings again (which exactly match the true signal wavelet here) and look at the MSE criteria for B=10 (`R=10`) bootstrap samples. Typically, a larger number of bootstrap samples is used, as these may be generated in parallel. We choose a lower number in the vignette for the sake of time.

```
set.seed(1414)
SNR10Boot <- WiSEBoot(SimulatedSNR1.0Series[ ,4], R=10)
SNR10Boot$MSECriteria
```

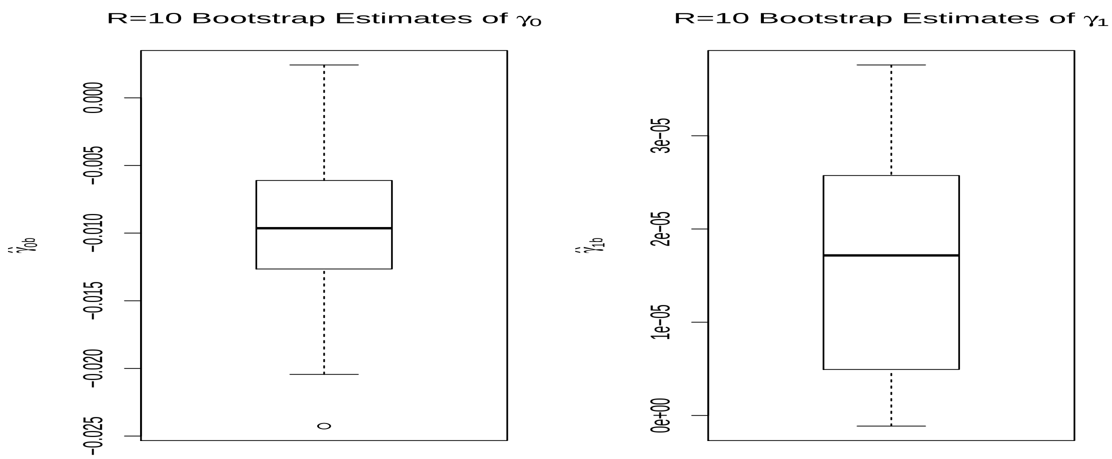
```
##       J0plusOne   meanOfMSE
##  [1,]         9 0.005253337
##  [2,]         8 0.004647180
##  [3,]         7 0.003526287
##  [4,]         6 0.002935839
##  [5,]         5 0.002609077
##  [6,]         4 0.002394103
##  [7,]         3 0.003768089
##  [8,]         2 0.004040207
##  [9,]         1 0.004421682
## [10,]         0 0.004503563
```

Even in this small bootstrap sample, the correct model was selected. We can see at $J_0 + 1 = 4$ the mean of the MSE is minimized with a value of 0.00239. The reader should keep in mind that this is a simulation example, so a desirable result is not surprising.

The output from `WiSEBoot` also may be used to examine the distributions of the γ_0, γ_1 and γ parameters, estimated by the bootstrap. The boxplots below show the parametric linear parameter estimates $(\hat{\gamma}_{0b}, \hat{\gamma}_{1b})$. Because the data was simulated, the population parameters are known to be $\gamma_0 = 0, \gamma_1 = 0$.

```
par(mfrow=c(1,2))
boxplot(SNR10Boot$BootIntercept,
        main=expression(paste("R=10 Bootstrap Estimates of ", gamma[0])),
        ylab=expression(hat(gamma)[0][b]))
boxplot(SNR10Boot$BootSlope,
```

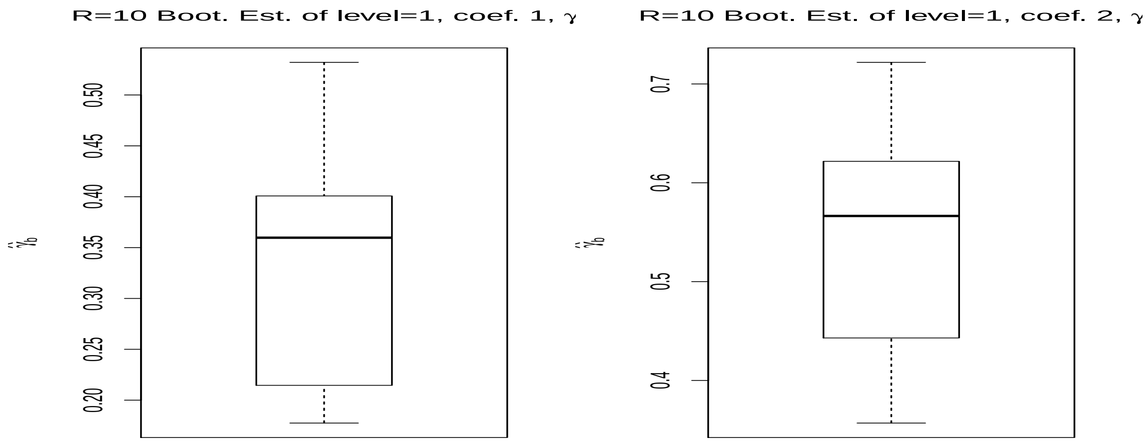
```r
       main=expression(paste("R=10 Bootstrap Estimates of ", gamma[1])),
       ylab=expression(hat(gamma)[1][b]))
```



As always in any type of bootstrap, the bootstrap distribution will be centered around the original estimate from the data. We can see that these boxplots aren't exactly centered at 0 because of this centering issue associated with the bootstrap.

If we wanted to look at the bootstrap distribution of any individual filter wavelet coefficient, the output from `WiSEBoot` also makes this possible. Below are the bootstrap distributions of the level=1 filter coefficients.

```r
par(mfrow=c(1,2))
boxplot(SNR10Boot$BootWavelet[,3],
       main=expression(paste("R=10 Boot. Est. of level=1, coef. 1, ", gamma)),
       ylab=expression(hat(gamma)[b]))
boxplot(SNR10Boot$BootWavelet[,4],
       main=expression(paste("R=10 Boot. Est. of level=1, coef. 2, ", gamma)),
       ylab=expression(hat(gamma)[b]))
```



3 WiSE Bootstrap Hypothesis Test

Next we provide a brief introduction to a hypothesis test of the wavelet coefficients from two data series of equal lengths. This hypothesis testing methodology is discussed in detail in (Braverman, 2015). This theoretical discussion is meant to give users of the `WiSEHypothesisTest` and `WiSEConfidenceRegion` a general idea of the methodology occurring.

Consider two equally-spaced data series of length $T = 2^J, J \in \mathbb{I}^+$. Each data series follows the model from eqn. 1. That is,

$$Y(t) = \gamma_{y0} + \gamma_{y1}t + W\gamma_y + e_y(t)$$

$$X(t) = \gamma_{x0} + \gamma_{x1}t + W\gamma_x + e_x(t)$$

Users of these functions wish compare the signals of these two series. Namely, the user may test the linear relationship between the two sets of wavelet coefficients: $\gamma_y = \alpha + \beta\gamma_x$. The null hypothesis in `WiSEHypothesisTest` is

$$H_0 : \alpha = m, \beta = n, \quad m, n \in \mathbb{R}$$

In Braverman, 2015, values of $m = 0$ and $n = 1$ are tested. If the null hypothesis in this specific scenario is not rejected, then we may say that signal within the climate model output matches the observed climate.

The algorithm to generate the WiSE bootstrap sample under the null hypothesis changes slightly. Please see (Braverman, 2015) for the details.

4 WiSE Bootstrap for Hypothesis Testing: Climate Model Signals

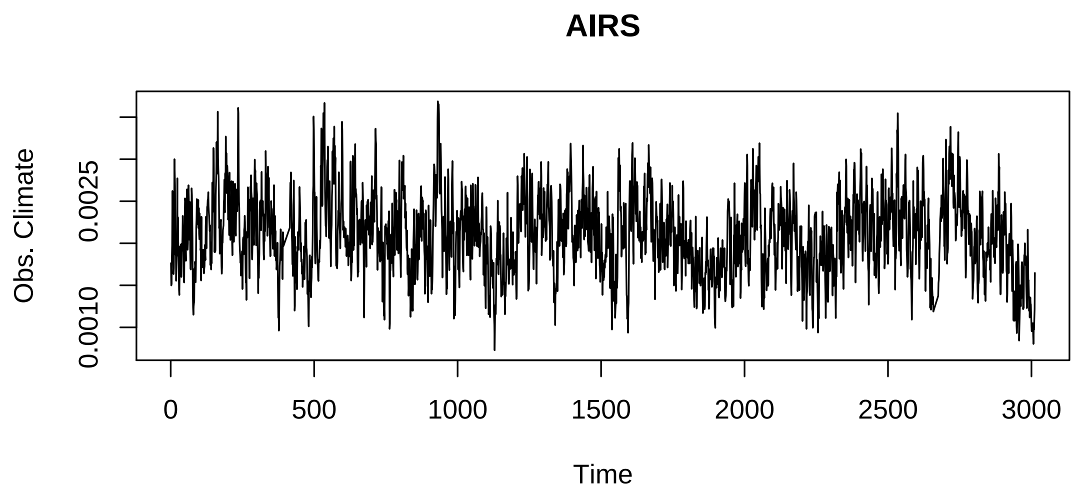
An example analysis of climate model data is presented here. The full analysis of the climate models at some specific grid-cells is available in (Braverman, 2015). Within the `WiSEBoot` package, two sets of climate model outputs and observed climate are available. Here, we will look at the data in `CM20N20S60E`.

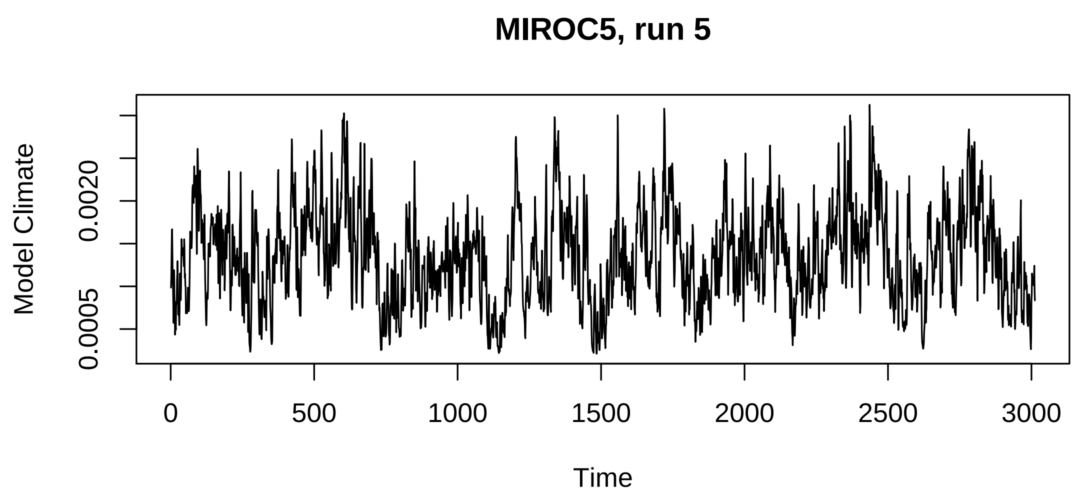
```
data(CM20N20S60E)
CM20N20S60E[1:3,]


##                   AIRS    IPSLRun1    IPSLRun2     IPSLRun3    IPSLRun4
## 2002-10-01 0.001764203 0.001844154 0.002112894 0.0006225206 0.001579949
## 2002-10-02 0.001498882 0.001700833 0.001708422 0.0006596091 0.001716239
## 2002-10-03 0.001522536 0.001539518 0.001419565 0.0008227325 0.001948907
##             MIROC5Run1   MIROC5Run2   MIROC5Run3  MIROC5Run4  MIROC5Run5
## 2002-10-01 0.001653560 0.0017041005 0.0010692392 0.001497587 0.000984715
## 2002-10-02 0.001490860 0.0011596567 0.0010018310 0.001331268 0.001106074
## 2002-10-03 0.001315217 0.0008881064 0.0008363572 0.001092815 0.001381810
##             MIROC5Run6
## 2002-10-01 0.001133758
## 2002-10-02 0.001047236
## 2002-10-03 0.001029497
```

This data matrix contains runs from AIRS (observed climate), 4 runs of the IPSL model, and 6 runs of the MIROC5 model. The model runs are obtained by choosing different starting parameters. This matrix contains a set of specific humidity observations/outputs between 20N and 20S at 60E and an altitude of 500 hPa. Observations are daily, from October 1, 2002 to December 29, 2010.

We'll specifically compare the signals in AIRS and MIROC5, run 5. Here are some plots of the raw data.

```
par(mfrow=c(2,1))
plot.ts(CM20N20S60E[,1], main="AIRS", ylab="Obs. Climate")
plot.ts(CM20N20S60E[,10], main="MIROC5, run 5", ylab="Model Climate")
```





Before it is possible to use any of the WiSE bootstrap methodology, the data must first be of length $T = 2^J$ for a positive integer, J. The raw data contains 3012 observations. Thus, we first use the `padMatrix` function to lengthen each series simultaneously.

```
pad60E <- padMatrix(CM20N20S60E)
dim(pad60E$xPad)


## [1] 4096   11
```

The code above uses the default options of padding at both sides of the data series by reflecting. The linear trend is not replaced (default) to the padded data matrix because we may easily input the estimated linear (parametric) parameters to the hypothesis testing function. This data is now of length 2^{12}.

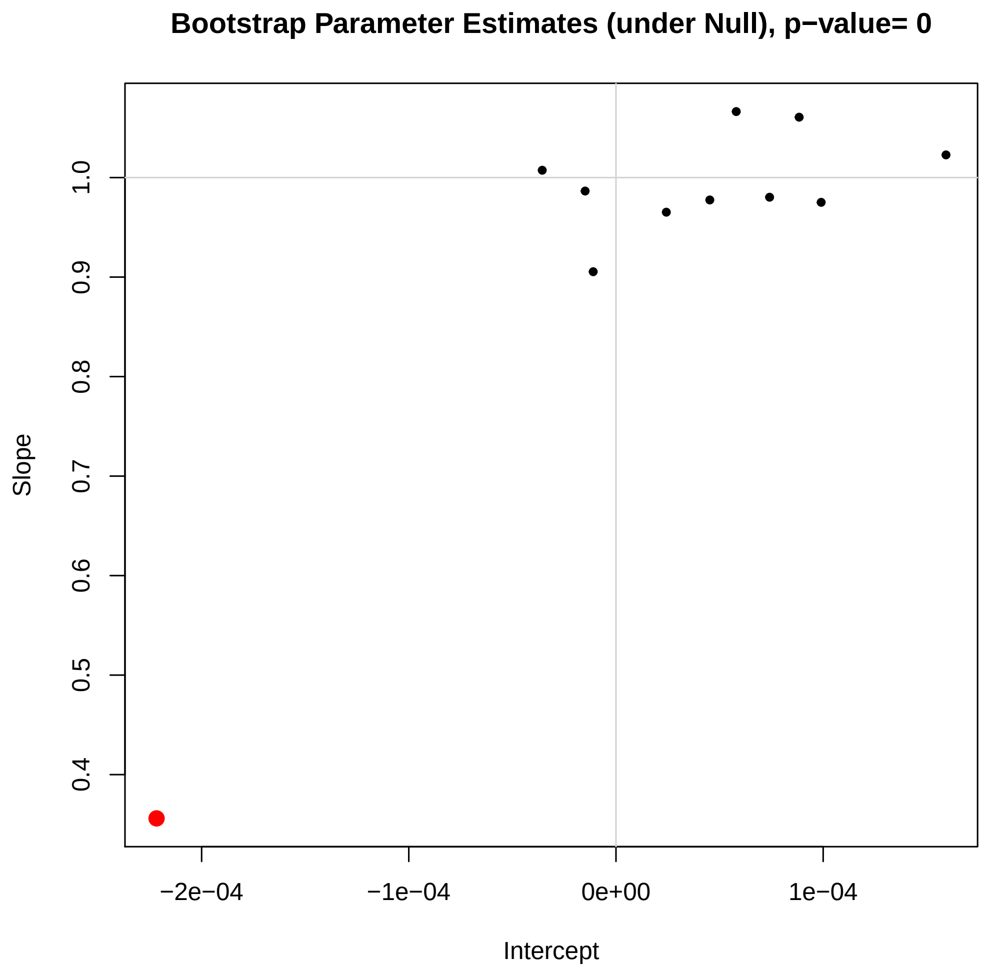
The hypothesis testing function requires that the user choose a wavelet coefficient threshold level. This may be done automatically with the `WiSEBoot` function, by inputting both series as a 4096 x 2 matrix. Here, we choose to use a threshold of $J_0 = 5$, as this corresponds to a cycle of 128 days.

Now that the data is of correct length, we may test the hypothesis

$$H_0 : \alpha = 0, \beta = 1$$

(i.e. the climate model signal matches the observed climate). Our 'X' series is AIRS and the 'Y' series is MIROC5, run 5. For demonstration purposes, we will choose to take `R=10` bootstrap samples. A higher number of samples is generally recommended.

```
hypObj <- WiSEHypothesisTest(pad60E$xPad[,1], pad60E$xPad[,10], R=10, J0=5,
                             XParam=pad60E$linearParam[,1],
                             YParam=pad60E$linearParam[,10])


## [1] "The asymptotic p-value is 2.11e-06.  The bootstrap p-value is 0"
```



The function prints two p-values. The asymptotic p-value is based upon the distribution of Hotelling's T^2 and the test statistic utilizes the variance-covariance matrix from the bootstrap sample. The bootstrap p-value computes a Hotelling's T^2 test statistic for each bootstrap sample, and the quantile of the data-based Hotelling's T^2 is computed from the bootstrap sample. A plot of the bootstrap sample and observed data parameter estimates is also generated optionally.

We can see that both the asymptotic and bootstrap p-values indicate that the null hypothesis should be rejected. This is not surprising based upon the generated plot. The $\hat{\alpha}$ and $\hat{\beta}$ estimated from the data (red point) is clearly outside of the cloud of bootstrap sample points (black). The gray vertical and horizontal lines represent the parameter values under the null hypothesis.

Acknowledgments

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References

Chatterjee, S. and Heyman, M. "WiSE Bootstrap for model selection", 2015 (in progress).

Braverman, A., Cressie, N., Chatterjee, S., et al. "Probabilistic Climate Model Evaluation", 2015 (in progress).