Hockey sticks, principal components, and spurious significance

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The "hockey stick" shaped temperature reconstruction of Mann et al. (1998, 1999) has been widely applied. However it has not been previously noted in print that, prior to their principal components (PCs) analysis on tree ring networks, they carried out an unusual data transformation which strongly affects the resulting PCs. Their method, when tested on persistent red noise, nearly always produces a hockey stick shaped first principal component (PC1) and overstates the first eigenvalue. In the controversial 15th century period, the MBH98 method effectively selects only one species (bristlecone pine) into the critical North American PC1, making it implausible to describe it as the "dominant pattern of variance". Through Monte Carlo analysis, we show that MBH98 benchmarks for significance of the Reduction of Error (RE) statistic are substantially under-stated and, using a range of cross-validation statistics, we show that the MBH98 15th century reconstruction lacks statistical significance. Citation: McIntyre, S., and R. McKitrick (2005), Hockey sticks, principal components, and spurious significance, Geophys. Res. Lett., 32, L03710, doi:10.1029/2004GL021750.

1. Introduction

[2] The term "hockey stick" is often used to describe the shape of the Northern Hemisphere (NH) mean temperature index introduced in Mann et al. [1998] (hereinafter referred to as MBH98). For convenience, we define the "hockey stick index" of a series as the difference between the mean of the closing sub-segment (here 1902–1980) and the mean of the entire series (typically 1400-1980 in this discussion) in units of the long-term standard deviation (σ), and a "hockey stick shaped" series is defined as one having a hockey stick index of at least 1 σ . Such series may be either upside-up (i.e., the "blade" trends upwards) or upside-down. Our focus here is on the 1400-1450 step ("AD1400 step") of MBH98, because of controversy over early 15th century temperature reconstructions [McIntyre and McKitrick, 2003; M. E. Mann et al., Note on paper by McIntyre and McKitrick in Energy and Environment, unpublished manuscript, 2003, available at ftp://holocene.evsc.virginia.edu/pub/mann/ EandEPaperProblem.pdf, hereinafter referred to as Mann et al., unpublished manuscript, 2003]. Our particular interest in the performance of the Reduction of Error (RE) statistic arises out of that controversy. We also focus on the North American tree ring network ("NOAMER"), because the first principal component ("PC1") of this

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network has been identified as essential for controversial periods of the MBH98 temperature reconstruction [Mann et al., 1999, unpublished manuscript, 2003]. MBH98 has recently been criticized on other grounds in von Storch et al. [2004].

- [3] MBH98 used principal components (PCs) to reduce the dimensionality of tree ring networks and stated that they used "conventional" PC analysis. A conventional PC algorithm centers the data by subtracting the column means of the underlying series. For the AD1400 step highlighted here, this would be the full 1400–1980 interval. Instead, MBH98 Fortran code (ftp://holocene.evsc.virginia.edu/pub/ MBH98/TREE/ITRDB/NOAMER/pca-noamer) contains an unusual data transformation prior to PC calculation that has never been reported in print. Each tree ring series was transformed by subtracting the 1902-1980 mean, then dividing by the 1902-1980 standard deviation and dividing again by the standard deviation of the residuals from fitting a linear trend in the 1902-1980 period. The PCs were then computed using singular value decomposition on the transformed data. (The effects reported here would have been partly mitigated if PCs had been calculated using the covariance or correlation matrix.) This previously unreported transformation was recently acknowledged in the Supplementary Information to a Corrigendum to MBH98 [Mann et al., 2004], where they asserted that it has no effect on the results, a claim we refute herein.
- [4] PCs can be strongly affected by linear transformations of the raw data. Under the MBH98 method, for those series in which the 1902–1980 mean is close to the 1400–1980 mean, subtraction of the 1902–1980 mean has little impact on weightings for the PC1. But if the 1902–1980 mean is different than the 1400–1980 mean (i.e., a hockey stick shape), the transformation translates the "shaft" off a zero mean; the magnitude of the residuals along the shaft is increased, and the series variance, which grows with the square of each residual, gets inflated. Since PC algorithms choose weights that maximize variance, the method reallocates variance so that hockey stick shaped series get overweighted. In effect, the MBH98 data transformation results in the PC algorithm mining the data for hockey stick patterns.
- [5] In a network of persistent red noise, there will be some series that randomly "trend" up or down during the ending sub-segment of the series (as well as other sub-segments). In the next section, we discuss a Monte Carlo experiment to show that these spurious "trends" in a closing segment are sufficient for the MBH98 method, when applied to a network of red noise, to yield hockey stick PC1s, even though the underlying data gener-

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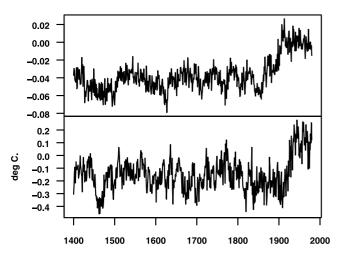


Figure 1. Simulated and MBH98 Hockey Stick Shaped Series. Top: Sample PC1 from Monte Carlo simulation using the procedure described in text applying MBH98 data transformation to persistent trendless red noise; Bottom: MBH98 Northern Hemisphere temperature index re-construction.

ating process has no trend component. We then examine the effect of this procedure on actual MBH98 weights for the North American PC1. Finally we use the simulated PC1s to establish benchmarks for the Reduction of Error (RE) verification statistic used by MBH98, and we discuss R² and other verification statistics for the MBH98 reconstruction.

2. Monte Carlo Simulations of Hockey Sticks on Trendless Persistent Series

[6] We generated the red noise network for Monte Carlo simulations as follows. We downloaded and collated the NOAMER tree ring site chronologies used by MBH98 from M. Mann's FTP site and selected the 70 sites used in the AD1400 step. We calculated autocorrelation functions for all 70 series for the 1400–1980 period. For each simulation, we applied the algorithm hosking.sim from the waveslim package version 1.3 downloaded from www.cran.r-project. org/doc/packages/waveslim.pdf [Gencay et al., 2001], which applied a method due to Hosking [1984] to simulate trendless red noise based on the complete auto-correlation function. All simulations and other calculations were done in R version 1.9 downloaded from www.R-project.org [R Development Core Team, 2003]. Computer scripts used to generate simulations, figures and statistics, together with a sample of 100 simulated "hockey sticks" and other supplementary information, are provided in the auxiliary material¹. We carried out 10,000 simulations, in each case obtaining 70 stationary series of length 581 (corresponding to the 1400-1980 period). By the very nature of the simulation, there were no 20th century trends, other than spurious "trends" from persistence. We applied the MBH98 data transformation to each series in the network: the 1902-1980 mean was subtracted, then the series was divided by

the 1902–1980 standard deviation, then by the 1902–1980 detrended standard deviation. We carried out a singular value decomposition on the 70 transformed series (following MBH98) and saved the PC1 from each calculation.

- [7] The simulations nearly always yielded PC1s with a hockey stick shape, some of which bore a quite remarkable similarity to the actual MBH98 temperature reconstruction as shown by the example in Figure 1. A sharp inflection was regularly observed at the start of the 1902–1980 "calibration period". Figure 2 shows histograms of the hockey stick index of the simulated PC1s. Without the MBH98 transformation (top panel), a 1 σ hockey stick occurs in the PC1 only 15.3% of the time (1.5 σ 0.1%). Using the MBH98 transformation (bottom panel), a 1 σ hockey stick occurs over 99% of the time, (1.5 σ 73%; 1.75 σ 21% and 2 σ 0.2%).
- [8] The hockey sticks were upside-up about half the time and upside-down half the time, but the 1902-1980 mean is almost never within one σ of the 1400-1980 mean under the MBH98 method. PC series have no inherent orientation and, since the MBH98 methodology uses proxies (including the NOAMER PC1) in a regression calculation, the fit of the regression is indifferent to whether the hockey stick is upside-up or upside-down. In the latter case, the slope coefficient is negative. In fact, the North American PC1 of *Mann et al.* [1999] is an upside-down hockey stick, as shown at ftp://ftp.ngdc.noaa.gov/paleo/contributions_by_author/mann1999/proxies/itrdb-namer-pc1.dat.
- [9] The loadings on the first eigenvalues were inflated by the MBH98 method. Without the transformation, the median fraction of explained variance of the PC1 was only 4.1% (99th percentile–5.5%). Under the MBH98 transformation, the median fraction of explained variance from PC1 was 13% (99th percentile–23%), often making the PC1 appear

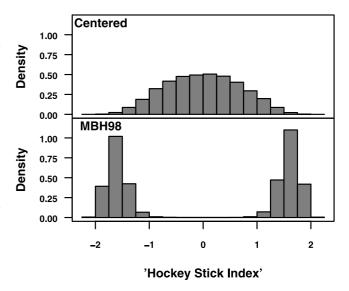


Figure 2. Histogram of 'Hockey Stick Index' for PC1s. For the 10,000 simulated PC1s described in text, the histogram shows the distribution of the difference between the 1902–1980 mean and the 1400–1980 mean, divided by the 1400–1980 standard deviation. Top: Conventional (centered) calculation; Bottom: with MBH98 data transformation.

¹Auxiliary material is available at ftp://ftp.agu.org/apend/gl/2004GL021750.

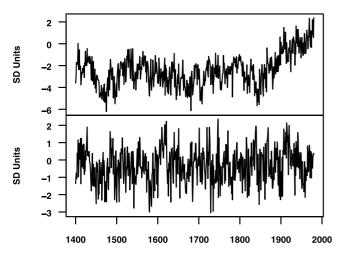


Figure 3. PC1 for AD1400 North American Tree Ring Network. Top: Result with MBH98 data transformation; Bottom: recalculated on the same data without MBH98 data transformation. Both standardized to 1902–1980 period.

to be a "dominant" signal, even though the network is only noise.

3. The PC1 in the MBH98 North American Network

- [10] We now show the effect of the MBH98 algorithm on the actual NOAMER network in the controversial AD1400 step.
- [11] Without the data transformation the PC1 is very similar to the unweighted mean of all the series and, as shown in the bottom panel of Figure 3, does not have a hockey stick shape. However, under the MBH98 algorithm, the PC1 has a marked hockey stick shape, as shown in the top panel of Figure 3. The MBH98 method creates a PC1 which is dominated by bristlecone pines and closely related foxtail pines. (Foxtail pines are located in an adjacent mountain range, interbreed with bristlecone pines and are included here with bristlecone pines collectively). Out of 70 sites in the network, 93% of the variance in the MBH98 PC1 is accounted for by only 15 bristlecone and foxtail pine sites

collected by Donald Graybill [Graybill and Idso, 1993] (see Table 1). The weights in the MBH98 PC1 have a nearly linear relationship to the hockey stick index. The most heavily weighted site in the MBH98 PC1, Sheep Mountain, is a bristlecone pine site with the most pronounced hockey stick shape $(1.6\,\sigma)$ in the network; it receives over 390 times the weight of the least weighted site, Mayberry Slough, whose hockey stick index is near 0.

- [12] Under the MBH98 data transformation, the distinctive contribution of the bristlecone pines is in the PC1, which has a spuriously high explained variance coefficient of 38% (without the transformation 18%). Without the data transformation, the distinctive contribution of the bristlecones only appears in the PC4, which accounts for less than 8% of the total explained variance.
- [13] This substantially reduced share of explained variance, together with the fact that species other than bristlecone/foxtail pines are effectively omitted from the MBH98 PC1, argues strongly against interpreting it as the "dominant component of variance" in the North American network (M. E. Mann et al., Reply to "Global-scale temperature patterns and climate forcings over the past six centuries: A comment" by S. McIntyre and R. McKitrick, unpublished manuscript, 2004, available at http://stephenschneider. stanford.edu/Publications/PDF Papers/MannEtAl2004.pdf). McIntyre and McKitrick [2005] discuss, inter alia, problems relating to the interpretation of bristlecone/foxtail pine growth as a temperature proxy, and we show the impact of using conventional (centered) PC methods on the MBH98 northern hemisphere temperature index, which has a significant effect on the relative values in the 15th and 20th centuries.

4. Benchmarking the Reduction of Error Statistic for the MBH98 Algorithm

[14] In most dendroclimatic studies several verification statistics are used. For example, *Cook et al.* [1994] describe the Reduction of Error (RE), R², Coefficient of Efficiency (CE), sign test and product mean tests as measures of skill. MBH98 only reported RE statistics to demonstrate statistical skill, reporting an RE value for their AD1400 step of 0.51. There is no theoretical distribution of the RE statistic

Table 1. 15 Highly Weighted Sites in MGH98 PC1^a

| ID Code | Name | Species | Elevation (m) | Author | Graybill and Idso [1993] # |
|---------|-------------------|---------|---------------|-------------------|-------------------------------|
| az510 | San Francisco Pks | PIAR | 3535 | D.A. Graybill | 10 |
| ca528 | Flower Lake | PIBA | 3291 | D.A. Graybill | 13 |
| ca529 | Timber Gap Upper | PIBA | 3261 | D.A. Graybill | 14 |
| ca530 | Cirque Peak | PIBA | 3505 | D.A. Graybill | 12 |
| ca533 | Campito Mountain | PILO | 3400 | D.A. Graybill | 5 |
| | • | | | and V.C. Lamarche | |
| ca534 | Sheep Mountain | PILO | 3475 | D.A. Graybill | 11 |
| co522 | Mount Goliath | PIAR | 3535 | D.A. Graybill | 2 |
| co523 | Windy Ridge | PIAR | 3570 | D.A. Graybill | 4 |
| co524 | Almagre Mountain | PIAR | 3536 | D.A. Graybill | 1 |
| co525 | Hermit Lake | PIAR | 3660 | D.A. Graybill | 3 |
| nv510 | Charleston Peak | PILO | 3425 | D.A. Graybill | 6 |
| nv512 | Pearl Peak | PILO | 3170 | D.A. Graybill | 9 |
| nv513 | Mount Washington | PILO | 3415 | D.A. Graybill | 8 |
| nv514 | Spruce Mountain | PILO | 3110 | D.A. Graybill | |
| nv516 | Hill 10842 | PILO | 3050 | D.A. Graybill | |

^a15 high-altitude bristlecone (PILO, PIAR) and foxtail (PIBA) sites dominating MBH98 PC1, constituting 13 of 14 sites listed in Table 1 of *Graybill and Idso* [1993].

and hence no exact or asymptotic tables of significance levels [*Cook et al.*, 1994]. MBH98 attempted to benchmark the significance level for the RE statistic using Monte Carlo simulations based on AR1 red noise with a lag coefficient of 0.2, yielding a 99% significance level of 0.0. However their simulation under-estimates the actual persistence of tree ring proxies and ignores the effect of the MBH98 data transformation in over-weighting hockey stick shaped series.

- [15] In order to obtain more accurate significance benchmarks, we regressed each of the 10,000 simulated PC1s against the MBH98 northern hemisphere temperature series (the "sparse" subset used by MBH98 for verification ftp:// ftp.ngdc.noaa.gov/paleo/paleocean/by contributor/ mann1998/nhem-sparse.dat) in the 1901-1980 calibration period – a procedure which more closely emulates actual MBH98 methods. Since the simulated PC1s are red noise series containing no information about the climate, they can be used to establish lower limits for the significance levels which the actual proxy data must exceed to indicate reconstructive skill. Since MBH98 used 22 indicators in their AD1400 step calculation, whereas the Monte Carlo simulation used only the simulated NOAMER PC1, the actual RE significance level would be higher than the benchmark calculated here, which is only a lower limit, making the arguments herein conservative.
- [16] For each regression, we calculated the temperature "reconstruction" from the simulated PC1 in the verification period (1854–1901), and used the "reconstruction" to calculate the RE, R², CE, Sign Test and Product Mean Test. From this data, we determined the 99% significance levels in the verification period as shown in Table 2. The pattern of verification statistics was quite consistent: a high RE statistic, a very low CE statistic and a low R² statistic, relative to white or weakly red noise values.
- [17] According to our calculations, the lower-limit critical value for 99% RE significance is 0.59 (5% 0.54), values much higher than the 99% critical value of 0.0 reported by MBH98. The reported RE value for the AD1400 step of the MBH98 reconstruction was 0.51 (90th percentile under our RE distribution). Mann et al. have not archived supporting calculations for the AD1400 step. Accordingly, we emulated the AD1400 step of MBH98 using their data, obtaining the verification period statistics shown in Table 3. We were only able to obtain an RE statistic of 0.46 (80th percentile under our RE distribution) and an R^2 statistic of 0.02 (statistically insignificant). Other verification statistics also lack statistical significance and the high RE-low R^2 pattern is obviously similar to the patterns from comparably treated red noise.

5. Discussion and Conclusions

[18] PC analyses are sensitive to linear transformations of data, even if such transformations only appear to be

Table 2. Statistical Significance Levels^a

| Verification Statistic | 99% Significance Level (Simulation) | 99% Significance Cutoff Used by MBH98 |
|---------------------------|-------------------------------------|--|
| RE (β) R ² | 0.59 | 0.00 |
| R^2 | 0.15 | 0.20 |
| CE | 0.03 | NA |
| Sign Test | 32 | NA |
| Product Mean Test | 2.73 | NA |

^a99% benchmarks from simulations described in text in and as reported by MBH98.

Table 3. Verification Period Statistics for AD1400 Step of MBH98 Reconstruction^a

| | AD1400 Step Results | | |
|--------------------------|---------------------|----------------|--|
| | Emulation | MBH98 Reported | |
| RE (β) | 0.46 | 0.51 | |
| RE (β) R ² | 0.02 | NA | |
| CE | -0.26 | NA | |
| Sign Test | 22 | NA | |
| Product Mean Test | 1.54 | NA | |

^aFrom emulation and as reported by MBH98.

"standardizations". Here we have shown, in the case of MBH98, that a "standardization" step (that the authors did not even consider sufficiently important to disclose at the time of their study) significantly affected the resulting PC series. Indeed, the effect of the transformation is so strong that a hockey-stick shaped PC1 is nearly always generated from (trendless) red noise with the persistence properties of the North American tree ring network. This result is disquieting, given that the NOAMER PC1 has been reported to be essential to the shape of the MBH98 Northern Hemisphere temperature reconstruction.

[19] For evaluation of statistical skill in paleoclimatic studies, the Reduction of Error (RE) statistic is widely used, but lacks a theoretical distribution. Practitioners use Monte Carlo models to establish significance benchmarks. Here we have shown that the benchmarks can be dramatically affected by the Monte Carlo model itself and that the 99% significance level from a Monte Carlo model more accurately representing actual MBH98 procedures is 0.59, as compared to the level of 0.0 reported in the original study. More generally, this example shows that changes in methodology will generally require new Monte Carlo modeling, that benchmarks carried forward from one methodology cannot necessarily be applied to a new methodology - even if the method changes may appear slight, and that great caution is required prior to concluding statistical significance based on RE statistics.

[20] An obvious guard against spurious RE significance is to examine other cross-validation statistics, such as the R² and CE statistics, as recommended, for example, by Cook et al. [1994]. While there are limitations to the R² statistic, the analysis of statistical "skill" of Murphy [1988] presupposes that the R² statistic exceeds the skill statistic and cases where the RE statistic exceeds the R² statistic are of particular concern [Cook et al., 1994]. In the case of MBH98, unfortunately, neither the R² and other cross-validation statistics nor the underlying construction step have ever been reported for the controversial 15th century period. Our calculations have indicated that they are statistically insignificant. Timely reporting of these statistics (in the original article) might have led to an earlier consideration of the discrepancy between the apparently high RE value and the low values of other statistics, and thus enabled earlier identification of the underlying data transformation resulting in this problem.

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