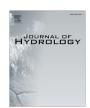
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Research papers

Prewhitening of hydroclimatic time series? Implications for inferred change and variability across time scales



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ABSTRACT

Prewhitening, the process of eliminating or reducing short-term stochastic persistence to enable detection of deterministic change, has been extensively applied to time series analysis of a range of geophysical variables. Despite the controversy around its utility, methodologies for prewhitening time series continue to be a critical feature of a variety of analyses including: trend detection of hydroclimatic variables and reconstruction of climate and/or hydrology through proxy records such as tree rings. With a focus on the latter, this paper presents a generalized approach to exploring the impact of a wide range of stochastic structures of short- and long-term persistence on the variability of hydroclimatic time series. Through this approach, we examine the impact of prewhitening on the inferred variability of time series across time scales. We document how a focus on prewhitened, residual time series can be misleading, as it can drastically distort (or remove) the structure of variability across time scales. Through examples with actual data, we show how such loss of information in prewhitened time series of tree rings (so-called "residual chronologies") can lead to the underestimation of extreme conditions in climate and hydrology, particularly droughts, reconstructed for centuries preceding the historical period.

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1. Introduction and objective

Prewhitening consists of fitting time series models such as autoregressive (AR) or autoregressive moving average (ARMA) models to an "original" time series and separating out the time series of residuals from the original series, which becomes the "prewhitened" series. The difference between the underlying original (presumably true) process and a prescribed model process will result in a realisation of "some" new process, which inherits "some" properties from the original process excluding (partly or fully) the short-term persistence, which was removed by fitting and effectively removing the AR or ARMA process. The question is whether or not the properties of the prewhitened series still carry the important information of interest embedded in the respective original time series, including signals at a range of frequencies (or time scales). The importance of this question cannot be understated, as the prewhitened or "residual" time series form the foundation for various types of analyses such as trend analysis and paleo-reconstruction based on dendrochronology and other proxy records.

In this paper, we investigate how prewhitening changes the properties of a time series in ways other than short-term persistence (i.e., the intended change). We assess the implications of prewhitening for our inferences on variability of time series across a range of time scales, which relates to the magnitude and significance of trends and cycles at different frequencies. For this purpose, we utilize examples based on long tree-ring time series, collected in the headwaters of Saskatchewan River Basin, Canada. that exhibit significant cross correlation with streamflows. The context and focus of this work is tailored to applications in reconstruction of paleo-climate and paleo-hydrology. However, our findings may also be of relevance for other types of analyses using prewhitening such as in trend detection of hydroclimatic variables with the Mann-Kendall and other tests (Bayazit and Önöz, 2007; Douglas et al., 2000; von Storch, 1995; Yue and Wang, 2002). We note that the analyses and implications discussed in this study are not intended to undermine the general utility of prewhitenning in the full range of its applications. Instead, this paper attempts to highlight some possible caveats and pitfalls that one might need to consider when using prewhitenning.

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2. Applications of prewhitening: The status quo

2.1. Prewhitening in trend analysis

Trend analysis of time series aims to identify a deterministic trend that has a physical basis and is likely to continue in the future. The Mann-Kendall (MK) trend test, named after Mann (1945) and Kendall (1975), is a widely used means for trend detection in a range of hydroclimatic and other variables. Ideally this test would only be used when there is a sound physical basis and understanding for the deterministic drivers that may be causing the trend. It is a rank-based nonparametric test with a null hypothesis that the time series under investigation has no trend (independent and identically distributed data), and with the alternative hypothesis that a monotonic (upward or downward) trend exists in the time series. An underlying assumption in this test is that the time series is not serially correlated, whereas this assumption is frequently violated in practice when dealing with hydroclimatic time series. A positive serial correlation increases the likelihood of rejecting the null hypothesis when it might be true (the probability of type 1 error would become larger than what the attained significance level indicates). Prewhitening was proposed by von Storch (1995) as a remedy to this issue, and since then has been used extensively with the MK test (Hamed, 2009: Lacombe et al., 2012: Zhang et al., 2000).

Yue et al. (2002) and Matalas and Sankarasubramanian (2003) examined the interaction between a linear trend and an AR(1) process and showed how the existence of serial correlation alters the variance of the estimate of the MK and linear regression tests, respectively. Yue and Wang (2002) asserted that the use of prewhitening with the MK test is based on an implied, but strong assumption that prewhitening could remove the AR process from a time series without affecting the existing trend, while it would seriously distort the test result. This led to a debate about the impact of prewhitening on trend detection and whether or not it should be applied (Bayazit, 2015; Bayazit and Önöz, 2007; Zhang and Zwiers, 2004). Yue and Wang (2002) showed that removing a positive AR(1) process will remove a portion of the underlying trend and hence reduce the likelihood of accepting the null hypothesis when it may be false (Type 2 error), thereby lowering the power of the test. Despite these implications, prewhitening continues to be a critical feature of trend analysis studies and the use of more advanced time series models, such as FGN, FARMA (Hamed, 2009) and ARIMA (Klaus et al., 2015), that possess longer term persistence are increasingly common.

2.2. Prewhitening in paleo-reconstruction

Reconstructions of paleo-hydroclimatic conditions, including past precipitation, temperature, and streamflow, can be derived from proxy records such as tree-ring widths. Tree rings archive information on annual (and sub-annual) hydro-climatic conditions across centuries, thereby providing a platform for characterizing change and variability in climate and hydrologic variables across time scales, from annual to multi-decadal. Exploiting the correlation between time series of tree-ring widths (detrended to remove age-related effects) and hydro-climatic variables is often the basis for reconstruction approaches. Reconstruction approaches typically employ multivariate statistical methods such as regression to relate one or more tree-ring time series, called "chronologies", to the climate/hydrologic variable of interest. These models are calibrated and tested on the common period of observational and proxy records and then used to reconstruct the past (Brockway and Bradley, 1995; Meko et al., 2012).

One challenge is that short-term persistence (here considered synonymous with an autoregressive correlation structure) in chronologies, is typically significantly higher than that of climatic or hydrologic variables (see Razavi et al., 2016 for discussion), due to biological carry-over effect of trees. Prewhitening was recommended by Cook (1985) to remove such short term persistence in tree-ring analysis, and since then, has been taught and used extensively to remove or diminish the inflated short-term persistence prior to paleo-reconstruction (e.g., Van Deusen, 1989; Axelson et al., 2009; Cleaveland and Duvick, 1992; Cleaveland and Stahle, 1989; Cook and Pederson, 2011; Fleming and Sauchyn, 2013; Gangopadhyay et al., 2009; Loaiciga et al., 1993; Maxwell et al., 2011; Meko et al., 2011; Meko et al., 2007; Sauchyn et al., 2011; Woodhouse et al., 2006; Woodhouse and Lukas, 2006b). The prewhitened time series, called "residual chronologies", are used as predictors to reconstruct a range of hydroclimatic variables, thereby informing water resources management, particularly about the past droughts (e.g., Woodhouse and Lukas, 2006a,b).

3. Structure of variability across time scales

The structure of variability across time scales (SVATS) herein refers to the way in which the variance (rate of variability) of a process changes with respect to changes in the time scale of analysis. Suppose k denotes the time scale in years and $\sigma^2(k)$ denotes the variance of a given time series (i.e., a realization of a process) at time scale k. For example, $\sigma^2(1)$ is the variance of the time series on the annual scale, $\sigma^2(2)$ is the variance of the two-year time series derived from that annual time series (by averaging every two consecutive years), and $\sigma^2(k)$ is the variance of its derived k-year-scale time series. When the number of data values in the annual time series is T (for T years), the number of data values in its two- and k-year-scale time series are T/2 and T/k. In general, the variance $\sigma^2(k)$ is expected to decrease as the time scale k increases. The rate and pattern of such a decrease in variance, however, are different for different geophysical time series.

3.1. Illustrative example

To illustrate the SVATS in time series, Fig. 1a and b show "variance vs. time scale" plots, on the log-log scale, for two different tree-ring time series (standard chronologies) called SFR and CAB for periods 1038-2008 and 1440-2003, respectively. These chronologies are located in Saskatchewan River Basin, Canada and exhibit significant positive correlations with their local streamflows. Details of these chronologies are available in Razavi et al. (2015). With no loss of generality, in this figure, all of the time series shown are standardized at the annual time scale (base time scale) so that they all have an annual variance of unity (i.e., $\sigma^2(1) = 1$). The points shown in Fig. 1 correspond to the behavior of the original time series and the residuals after fitting an AR(1), AR(3) and ARMA(1,1) model. The curves correspond to the AR(1), AR(2), AR(3), and ARMA(1,1) models fitted to the original time series. Section 3.2 presents the modelling details, and Section 3.3 discusses the properties of the resulting residuals.

Evidently in both cases, $\sigma^2(k)$ of the original time series decreases with the increase in k at rates smaller than that of a purely random process (i.e., white noise). This behaviour is a manifestation of the stochastic structure as a function of time scale (irregular long-term changes and trends at a range of frequencies). Such difference from a random process is also commonly attributed to persistence in geophysical time series at a range of time scales, particularly long-term persistence and the "Hurst Phenomenon" (Hurst, 1951; Klemeš, 1974; Mudelsee, 2007; Salas et al.,

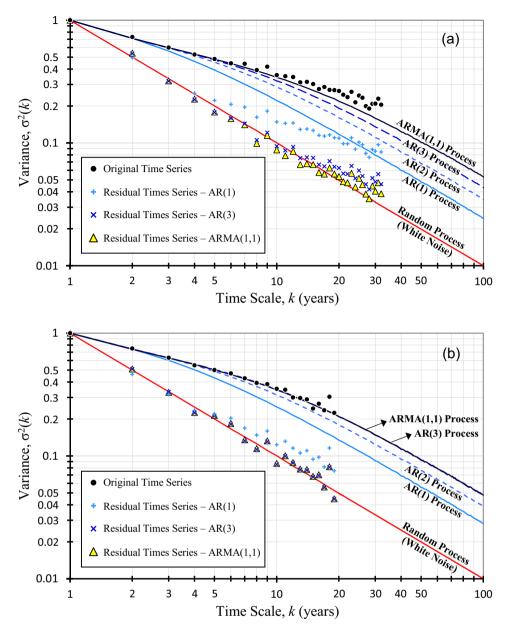


Fig. 1. "Variance vs. time scale" plots with original and residual time series of (a) SFR and (b) CAB tree-ring chronologies. The fitted AR and ARMA processes are shown by curves.

1979). The slope of a line passing though the points (not shown here) on the variance vs. time scale plot is known to be 2H-2, where H is called the "Hurst exponent" and is 0.5 for white noise (see Beran, 1994, page 92).

3.2. Performance of AR and ARMA models in reproducing SVATS

AR models are models of short-term persistence with a memory length controlled directly by the model order. Because of their short memory length, these models have been commonly assumed to be appropriate to capture and remove short-term persistence (autocorrelation) in time series. To generate the curves representing the AR and ARMA processes on Fig. 1a and b, we fitted AR(p) and ARMA(p,q) models to the time series, with p ranging from 1 to 6 and q = 1 (using SAMS software, Sveinsson et al., 2007), and used the corrected Akaike Information Criterion (Hurvich and Tsai, 1993) for their ranking;

accordingly, ARMA(1, 1) and AR(3) were the best and second best models for both of the time series.

Evidently, the different AR and ARMA processes can reproduce the underlying SVATS in the time series at different time-scale ranges from multi-annual to multi-decadal and longer, depending on their orders (i.e., the values of p and q). For example, AR(1) can accurately reproduce the underlying structure of variability up to approximately ~5-year scale, while for larger time scales, the rate of decrease in variance approaches that of a random process. However, AR(3) and ARMA(1,1) can reproduce the structure of variability for a wide range of time scales (even multi-decadal). Stated differently, a visual inspection of the plot suggests that, in these cases, the slope of AR(1) asymptotically approaches that of the random process between 5- and 10-year time scales, AR(2) does so between 10- and 20-year time scales, and AR(3) and ARMA(1,1) do so at time scales of greater than 20 years. We note that AR and ARMA processes with higher orders can reproduce this SVATS even at longer time scales (not shown).

3.3. SVATS in prewhitened time series

We showed above that the AR and ARMA models are capable of capturing and reproducing SVATS across a range of time scales. This capability directly affects the resulting prewhitened time series and limits the statistical properties that the prewhitened (residual) time series will inherit from the original time series. To assess how and to what extent the resulting residual time series preserve the SVATS of the respective original time series, let's look at the points already shown on Fig. 1a and b that represent residual time series resulting from fitting the AR(1), AR(3), and ARMA(1, 1) processes. As can be seen, the SVAT within the residual time series are drastically distorted or completely lost in the time-scale range shown. Such a loss of variance corresponds to a complete loss in information to the extent that the variability of the residual time series obtained from AR(3) and ARMA(1.1) is guite similar to that of a random process (no signal). This suggests that the effect of prewhitening on the residual time series goes well beyond removing short-term persistence (auto-correlation) as is so often assumed (see Section 2).

4. Implications and discussion

The possible distortion or loss of the SVAT can have serious implications that risk the credibility of any resulting statistical inferences performed on the residual time series. To further clarify these implications, we provide an alternative representation of the behaviour shown in the previous section. Fig. 2a shows the original SFR time series along with the respective residual time series obtained by fitting an AR(3) model – both of the time series are standardized to have identical average and variance at the annual time scale. This figure also shows 15- and 50-year moving average time series of the annual time series. Fig. 2b focuses on a subperiod (1600–2000) of Fig. 2a to better visually compare the original and residual time series at the annual time scale. Although the original and residual time series at the annual time scale possess

identical variance and may seem consistent with each other over time, their respective moving averages are significantly different. In other words, there is a significant reduction in information resulting from the removal of irregular trends and cycles in the residual time series as a result of the removal of the persistent component. The difference is particularly significant in the periods of consecutive dry or wet years (e.g., see periods 1460–1520 and 1650–1700). This indicates that the residual time series significantly underestimates the duration and extent of extreme (dry or wet) periods.

Fig. 2c and d compare the cumulative distribution functions (CDFs) of the original and residual time series at the annual and 15-year time scales, respectively. The annual-scale CDFs of the two time series are alike. On the 15-year time scale, however, the CDFs of the two are significantly different - the residual time series possesses only about *one quarter* of the variability of the

original time series at the same time scale
$$\left(\frac{\sigma_{residual}^2(15)}{\sigma_{original}^2(15)} = \frac{0.07}{0.28} = 0.25\right)$$
.

We note that the implications shown in the analyses above are general and can be seen for any other time series. This may have significant implications for the reconstruction of paleo-hydrology. The point is any reconstruction of climate or hydrologic variables for the centuries preceding the historical period inherits the statistical properties (including the SVATS) from its predictors. Therefore, if such residual time series ("residual chronologies") are used, the resulting reconstructions or inferences can be misleading, in particular in terms of the magnitude of extreme events – e.g., the magnitude of extreme droughts would be underestimated.

In the context of trend analysis, the observations in Fig. 2 reinforce the need to carefully distinguish the effects of trends and auto-correlation in trend detection. Yue et al. (2002) suggested the removal of a trend component from a time series prior to prewhitening as a first step and then adding the trend back to prewhitened time series for the Mann-Kendall test. This approach has been frequently used in the literature as a way to separate the two effects. It often requires the user to pre-specify a form for a

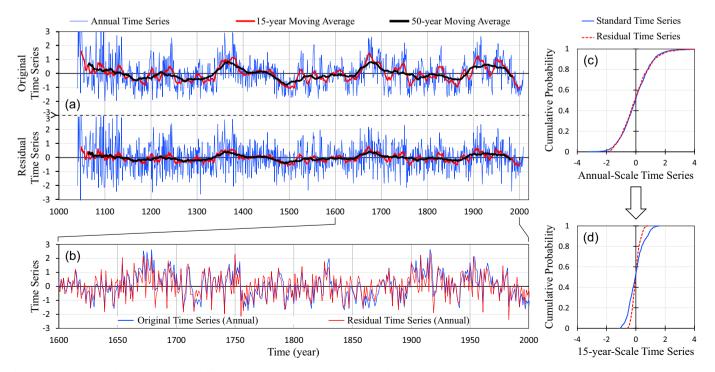


Fig. 2. (a) The original and residual time series of the SFR chronology along with their 15- and 50-year moving average time series. (b) The original and residual time series shown in (a) for sub-period 1600–2000. (c) The cumulative distribution functions (CDFs) of the original and residual time series. (d) The CDFs of the same time series at the 15-year time scale. The annual original and residual time series were standardized so that they have identical average of zero and variance of unity.

presumably existing trend, e.g., linear or other monotonic forms, which could lead to problems if there is no actual trend.

A deeper question underpinning our analysis would ask what information can a residual time series be expected to provide? In an ideal world where the correct form of the time series model is known, the resulting prewhitened residual time series based on that model would be a white noise exhibiting no information resulting from a deterministic process, whatsoever. In the real world, however, prewhitened residual time series represent only that portion of the original time series which cannot be described by the assumed time series model used to create those residuals. Alternatively stated, the possible existence of "some" information (signals) left in prewhitened time series is due to the inability of the assumed time series models to perfectly describe the underlying deterministic processes exhibited within the data. The message is that the quality and quantity of such information depend on the model used and cannot be easily interpreted especially for complex time series models. In spite of this, there are examples in the literature that used more complex models which exhibit longer memory, such as autoregressive integrated moving average (ARIMA) and fractional Gaussian noise (FGN) models, for prewhitening. Lastly, the autocorrelation structure of geophysical variables may be significantly non-stationary (Razavi et al., 2015). Such possible non-stationary behavior further complicates the impact of any prewhitening process that assumes a stationary process in original time series.

The variance vs. time scale plot shown in Fig. 1 is a powerful tool to investigate the serial dependencies in time series across the range of time scales. Using this tool, Fig. 3 compares the behaviour of 15 time series of tree growth rates (chronologies) and naturalized river flow in the Oldman River (a tributary of Saskatchewan River), Canada, over the historical period (1912–2001). The maximum time scale considered on the abscissa of Fig. 3 is short (8 years) relative to the much longer time scale considered in Fig. 1, because the length of the time series in Fig. 3 is relatively short (89 years). The short lengths of record associated

with the series in Fig. 3 result in much more scatter than was observed for the much longer time series used to develop Fig. 1.

As expected in Fig. 3, the variance decreases as the time scale increases for all the time series, however, the slope of the linear function that is fit to the tree-ring and streamflow series are quite different. The difference in slope at a time scale is attributable to the difference in persistence within the time series at that time scale, though these differences are also confounded by the short record lengths, somewhat. As can be seen, for short time scales (shorter than 3 years), the slopes of the two (flows and growth rates) are considerably different, with a slope associated with the flows closer to that of a random process, whereas for long time scales (longer than 3 years), the slopes of the two series are similar. This observation indicates that the short-term persistence in growth rates is higher than that of the flows (due to biological effects in trees), while the two are very similar in terms of their long term variability.

The result in Fig. 3 suggests that although standard chronologies do not properly represent the short-term persistence (autocorrelation) of hydro-climatic variables at the annual scale, they may exhibit an adequate representation of persistence and variability at longer time scales (2- or 3-year time scales and longer). This is due to the reduction of the carry-over effects associated with the growth of trees at longer time scales. As a result of this finding, instead of the conventional approach, we recommend focusing initial attention on reconstructing paleo-time series at multi-year time scales (e.g., 2- or 3-year time series instead of annual time series) and then disaggregating them into the annual time scale guided by the annual variability information in the tree-ring time series. See the initial attempt described by Razavi et al. (2016) for more analysis and discussion of the challenge of reconstructing multiyear scale paleo-hydrologic series. Razavi et al. (2016) showed that not only can this approach better represent the underlying SVATS, but also has a higher reconstruction power which explains a higher percentage of the variance in the hydro-climatic variable of interest than the series based on shorter time scales.

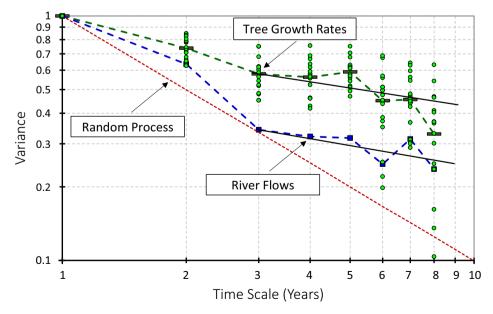


Fig. 3. Variance vs. time scale plot for flows in the Oldman River (square markers) and growth rates (circle markers) at 15 chronologies located in the Oldman basin over the historical period (1912–2001) – the solid lines are fitted by linear regression to the data of the time scale of three years and longer the plot is adopted from Razavi et al. (2016).

5. Final remarks

Since the recommendation by Cook (1985) to use prewhitening to remove short term persistence from long records of tree rings. prewhitening of hydroclimatic time series has proliferated in both courses and research as the solution to remove or diminish the impact of short-term persistence prior to paleo-reconstruction (see citations in Section 2). We have provided evidence and reasoning which documents why focusing one's attention on prewhitened hydroclimatic time series can be misleading, because it leads to a loss of important information contained in a time series. We have documented that prewhitened time series will generally not carry important stochastic properties embedded in respective original time series resulting from persistence and seasonality, and thus cannot preserve the SVATS (structure of variability across time scales). It was shown that prewhitening has impacts which may go well beyond the intended goal of only eliminating/reducing short-term persistence, and in fact, prewhitening distorts our ability to detect trends and cycles in time series and can also diminish their magnitude and significance. This is very important, as hydroclimatic time series possess a multitude of irregular trends and cycles at a range of frequencies and such information are essential for a variety of studies, in particular those relating to water resource management. The implications of prewhitening are of course different for different applications, and this paper suggests that the analyst be mindful of potential implications discussed.

Perhaps the most important negative implications of prewhitening are for paleo-reconstruction, where the prewhitening leads to a distortion of the time series which is then be transferred directly to the reconstructed time series of hydroclimatic variables. This indicates that resulting statistical inferences concerning paleo climatic conditions may not be credible and/or should be interpreted with caution. For example, the magnitude and duration of paleo-extremes such as droughts can be significantly *underestimated*, when prewhitened time series are used for hydroclimatic reconstruction. Note that the amount of the information loss due to prewhitening for a given time series depends on the extent of its SVATS (significance of signals at different frequencies) and the time series model used, and therefore, can be variable from one case study to another.

Although the phenomenon of inflated short-term persistence in tree-ring records (standard chronologies) appears to persist in recent literature (see citations in Section 2), it does not necessarily undermine the value of paleo-reconstructions based on standard chronologies. To address concerns over the fact that annual records of numerous geophysical records exhibit short-term persistence, an alternative would be to perform analysis over longer-time scales (e.g., two or three year time series) to effectively remove some of the short term persistence (see the approach proposed in Razavi et al., 2016). Tools such as those illustrated in the examples provided in Fig. 1 provide a generalized approach to exploring the impact of a very wide range of stochastic structures of short- and long-term persistence on the variability of hydroclimatic records.

In addition, future studies should consider the use of long "pseudo-proxy" data obtained from climate model simulations over the past millennium which may be useful in further characterizing the SVATS in climatic time series and the implications of prewhitening. Such data can be used in the evaluation of the performance of paleo-reconstruction methods, using controlled and systematic experiments known as pseudoproxy experiments (Smerdon, 2012).

Lastly, the analyses and implications discussed in this study were not intended to undermine the general utility of prewhitenning in the full range of its applications (including trend detection). Instead, this paper attempted to highlight some possible caveats

and pitfalls that one might need to consider when using prewhitenning in an application.

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