Supplementary Information

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Metrics to Quantify Anomaly Persistence of Soil Moisture (APSM)

The following criteria are typically used to test the short- and long-term persistence of a time series.

a) Length-of-runs (Gold test)

The probable number of runs of length n of N events in a series in which there is no persistence is usually examined using Gold's test [*Gold*, 1929]:

$$Q = \sum_{n=1}^{n'} \frac{(m''(n) - E[m''(n)])^2}{E[m''(n)]} \tag{A-1}$$

where Q is distributed as chi-square with (n'-1) degree of freedom, n' is the maximum run length in the series, and E[m"(n)] is the expected number of runs of n dry periods in a series of N years. Given that the dry ($\theta < \theta_{cl}$), normal ($\theta_{cl} < \theta < \theta_{cu}$), and wet ($\theta > \theta_{cu}$) periods occur independently with unequal probabilities p, q, and r, respectively, the E[m"(n)] in a series of N years for a purely random process is determined as below:

$$E[m''(n)] = 2p^2(q + r) + (N - n - 1)p^n(q + r)^2 \tag{A-2}$$

After determining Q, its significance is tested by comparison with the chi-square values obtained from tables. If the calculated value of Q is smaller than the chi-squared value obtained from tables with 95% probability, then the hypothesis that the sequence results from a purely random process is accepted.

b) Chi-square

Oladipo and Hare [1986] examined the tendency for persistence from year to year by constructing contingency tables indicating the distribution of the three categories of moisture conditions (dry, normal, and wet) for the previous and the following years for independence with the Fisher exact permutation test. In this context, and to check whether the triple classification scheme for moisture is independent, one can use the algorithm of *Pagano and Halvorsen* [1981].

c) Autocorrelation test

Oladipo and Hare [1986] also used log-one autocorrelation to examine the short-term dependence in time series which is usually measured by the magnitude of the low-order correlation coefficient. For this aim, the estimator recommended by *Jenkins* [1968] is used which computes as:

$$r_1 = \frac{\sum_{i=1}^{n}(x_i - \bar{x})(x_{i+1} - \bar{x})}{\sum_{i=1}^{n}(x_i - \bar{x})^2} \tag{A-3}$$

where n is the length of time series, x_i is the periodic (daily, monthly, seasonal, etc.) mean of the soil moisture of the i^{th} period, and

$$\bar{x} = \frac{1}{n}\sum_{i=1}^{n} x_i \tag{A-4}$$

After determining r_1, its significance is tested according to the following criteria the confidence level:

$$r_1 = \frac{-1 \pm z_a(n-2)^{\frac{1}{2}}}{n-1} \tag{A-5}$$

where z_a is the standard normal variate corresponding to a probability level *a*.

Similarly, *Liu and Avissar* [1999] used one-month-lag autocorrelation as a basic index to estimate the magnitude of persistence, expressed as

$$r(\tau) = \sum_{k=1}^{N-\tau} \frac{(x_k - \bar{x})(x_{k+\tau} - \bar{x})}{\sigma^2} \tag{A-6}$$

where τ is the lag length (in months) (assumed to be equal to 1), N is the length in months of the simulated time series of variable x_k (k=1,…, N) that is the monthly anomaly of the considered variable (i.e. soil moisture) with respect to its multiple-year average and $\bar{x}$ and σ^2 are its mean and variance.

d) Significant test of runs

Stahle and Cleaveland [1988] used a significant runs test to examine the presence of interannual persistence of growing season and June moisture anomalies in Texas. To this end, they first classified years into wet and dry years using the Palmer Drought Severity Index (PDSI), with years with a PDSI ≥ +2 classified as wet years and PDSI ≤ -2 classified as dry years. Then, the expected number of runs and the variance of a given category (e.g., PDSI ≥ +2 by PDSI ≥ +2 or PDSI ≤ -2 by PDSI ≤ -2) are determined using the following equations.

$$E_0(T) = \frac{M(M-1)}{N} \tag{A-7}$$

$$V_0(T) = \frac{M(M-1)}{N} \times \left[1 + \frac{(M-1)(M-2)}{N-1} - \frac{M(M-1)}{N}\right] \quad \text{(A-8)}$$

where E_0 is the expected value in a random normal distribution, V_0 is the variance of expected occurrence in the number of runs (T), T is the number of runs of a specific category (PDSI ≥ +2 after PDSI ≥ +2 or PDSI ≤ -2 after PDSI ≤ -2), M is the total number of occurrences of a category in a series, and N is the number of years in the series. After determining E_0 and V_0, the significance test of the runs is performed as follows.

$$z_0 = \frac{T - E_0(T)}{\sqrt{V_0(T)}} \quad \text{(A-9)}$$

where z_0 is the z-score and its significance level can be tested using the z-table. The null hypothesis is that given the number of times a condition occurs in a period; the times of occurrence are completely random.

e) Stored precipitation fraction (F_p)

McColl et al. [2017] defined fraction of stored precipitation (F_p) as the average fraction of precipitation that falls on a soil layer and is still available in the soil layer after 1/f days. One can calculate F_p as the integration of the positive soil water increments normalized by the total precipitation that falls during a given time period [*McColl et al.*, 2017]:

$$F_p(f) = \frac{\Delta z \sum_{i=1}^{fT} max\,(0, \Delta\theta_{i+})}{\int_0^T P(t)dt} \quad \text{(A-10)}$$

where θ and P represent soil moisture content and precipitation, respectively, and $\Delta\theta_i = \theta_i - \theta_{i-1}$, Δz determines soil layer depth and $\int_0^T P(t)dt$ determines accumulated precipitation (mm) throughout the study period. Precipitation, lateral flow, subsurface flow, capillary rise, etc., could lead to a positive increase in soil moisture [*Martínez-Fernández et al.*, 2021]. However, processes other than precipitation are assumed to be negligible.

f) Mean persistence time scale

The mean time spent continuously above or below a soil moisture threshold is also a criterion used to quantify the time scale of persistence [*Ghannam et al.*, 2016; *McColl et al.*, 2017]. Based on this criterion, the timescale of persistence is a period following an anomaly in which all elements of the series have the same sign as the anomaly [*Liu and Avissar*, 1999]. This period can be determined in the following steps [*Liu and Avissar*, 1999]: 1) take the time series of soil moisture and determine the anomalies in the data, 2) count the number of time steps that follow (e.g., months for monthly data) for a first non-zero $x_k(k = k_1)$ to $x_k(k = k_2)$ whose next element changes sign and set it as l_1, 3) count the following time steps for $x_k(k = k_2 + 1)$ to $x_k(k = k_3)$ whose next element changes sign again and set it as l_2, 4) repeat the procedure over the whole time series except for the last year, 5) take the average of l_1, l_2, ..., l_n as a measure of the time scale of persistence. If x_{k1} and x_{k2} have different signs, then $l_i = 0$. Therefore, it is likely to find an average of l_1, l_2, ... that is smaller than 1-time step.

g) Interannual mean-persistence time scale

This method is similar to the previous one except that persistence is determined for each day of year among all years. To this end, *Orth and Seneviratne* [2013] propose to proceed as follows: (1) calculate the mean and standard deviation (σ) of soil moisture data for each individual day of the year, considering data from all years for that day; (2) consider days falling within the range of mean $\pm$ σ as normal, within the range of mean $\pm$ 1.33σ as the first threshold for moderate anomalies, and in the range of mean $\pm$ 1.66σ as the second threshold for severe anomalies; (3) select all days in the time series between a given time period (e.g., summertime or full year) that exceed a threshold and calculate the delay before soil moisture returns to normal conditions; (iv) average all durations to derive a mean persistence of anomalous conditions once they have exceeded a certain threshold.

h) Hurst exponent

Unlike other previously defined metrics, *Shen et al.* [2018] used the Hurst exponent (H) [*Hurst*, 1951] to determine the presence of long-term persistence (also known as long-range correlation and long-term memory) or anti-persistence in soil moisture time series. Depending on whether soil moisture data exhibit long-term persistence or anti-persistence, the corresponding time window sizes were defined as the corresponding time scale. The approach takes advantage of the fact that soil moisture time series can be viewed as a $1/f^{2H+1}$ process (where f is the frequency and $0<H<1$ is the Hurst exponent), with an important subclass of those with long-term persistence (or long-term memory) [*Gao et al.*, 2006]. In other words, the $1/f^{2H+1}$ processes exhibit long-term persistence when $0.5<H<1$, anti-persistence when $0<H<0.5$, and memoryless behavior (or only short-term correlation) when H = 0.5 [*Gao et al.*, 2006]; *Shen et al.* [2018]. The latter (process with H = 0.5) is also referred to as the geometric random walk process.

Although numerous methods have been developed to date to determine the H exponent, such as rescaled range analysis, divergent fluctuation analysis, and adaptive fractal analysis (AFA), [*Shen et al.*, 2018] relied on the AFA method because it is superior to other methods in that it can handle arbitrary and strong nonlinear trends and more accurately estimates the Hurst exponent [*Riley et al.*, 2012]. Starting with the classical framework for the estimation of H, the variance of a given time series [X_t, t = 1,2…, N] for an arbitrary lag (donated as τ) is expressed as below

$$\sigma^2(\tau) = \frac{\sum_{t=1}^{N}(X_{t+\tau} - X_t)^2}{N} \tag{A-11}$$

For a random walk process, which is also known as geometric Brownian motion which has no autocorrelation, the variance varies linearly with lag, $\sigma^2(\tau)\sim\tau$. However, for processes where autocorrelation exists (processes that deviate from a random walk), the relationship between the variance for a given lag and the lag itself takes the following form:

$$\sigma^2(\tau)\sim\tau^{2H} \tag{A-12}$$

where H stands for the Hurst exponent. Performing the above calculations for multiple lag values, one can plot a linear line between $log\ \sigma^2(\tau)$ versus log τ and set the intercept to zero to determine H from the slope value.

Through the AFA method, the first step is to identify a globally smooth trend signal [v(i), i = 1, 2..., N] that must detrend the original data [u(i), i = 1,2..., N] where N is the length of the original data. The synthetic signal is created by merging the local polynomial fits with the original data. To do this, the original data u(i) must be divided into windows of length w = 2n+1, where the windows overlap by n+1 points, where n = (w-1)/2. Then, the best-fitting linear or quadratic polynomial is determined for each window. Standard least squares regression can be used for this purpose. When local fits are obtained for each window, they should be stitched to obtain a smooth global fit for the original time series. For stitching local fits, a weighted combination of the fits of overlapping points of two adjacent regions must be considered [*Riley et al.*, 2012]:

$$y^{(c)}(l) = w_1 y^{(j)}(l+n) + w_2 y^{(j+1)}(l), \quad l = 1,2,\dots,n+1, \qquad j = 1,2\dots,\frac{N}{n} - 1 \tag{A-13}$$

where $y^{(c)}$, $y^{(i)}$ and $y^{(i+1)}$ donate for combined, first, and adjacent locals, respectively, and $w_1 = \left(1 - \frac{l-1}{n}\right)$ and $w_2 = \frac{l-1}{n}$. After generating the global smooth trend signal, the next step is to detrend the original time series using this synthetic signal:

$$y(i) = u(i) - v(i) \tag{A-14}$$

The above steps should be repeated for a range of w values between 3 and N/2. Then, for each window size of w, the variance of the residuals should be determined as follows:

$$F(w) = \left[\frac{1}{N}\sum_{i=1}^{N}(u(i) - v(i))^2\right]^{1/2} \tag{A-15}$$

For fractal processes, F(w) then scales with w as follows:

$$F(w) \sim w^H \tag{A-16}$$

Finally, the above equation can be linearly derived to determine the exponent H.

i) Persistence duration of soil moisture difference

Song et al. [2019] argued that the lag correlation used for both SMM and APSM calculations neglects SMM variations caused by atmospheric forcing in each area, does not account for the nonlinear processes in APSM, and assumes that the data are stationary even though most meteorological and hydrological processes are not. Therefore, to overcome these limitations, they proposed to quantify the length of the memory using the persistence duration of the difference in soil moisture between the control experiment and the sensitivity experiment, requiring a series of experiments with a control experiment and one or more sensitivity experiments. The initial soil moisture in the control experiment is set to the observed soil moisture values and a fraction of the observed values is used for the sensitivity experiments. However, it can be argued that the proposed method can be accurate if it is ensured that there is no memory in the control experiment, while this cannot be guaranteed for the proposed method that uses measured soil moisture data and that therefore needs to be adjusted for further use.

References

Gao, J., et al. (2006), Assessment of long-range correlation in time series: how to avoid pitfalls, *Physical Review E*, *73*(1), 016117.

Ghannam, K., et al. (2016), Persistence and memory timescales in root-zone soil moisture dynamics, *Water Resources Research*, *52*(2), 1427-1445.
Gold, E. (1929), Note on the frequency of occurrence of sequences in a series of events of two types, *Quarterly Journal of the Royal Meteorological Society*, *55*(231), 307-309.
Hurst, H. E. (1951), Long-term storage capacity of reservoirs, *Transactions of the American society of civil engineers*, *116*(1), 770-799.
Jenkins, G. M. (1968), Spectral analysis and its applications, *Holden-Day, Inc., San Francisco, Card Nr. 67-13840*.
Liu, Y., and R. Avissar (1999), A study of persistence in the land–atmosphere system using a general circulation model and observations, *Journal of climate*, *12*(8), 2139-2153.
Martínez-Fernández, J., et al. (2021), Soil moisture memory and soil properties: An analysis with the stored precipitation fraction, *Journal of Hydrology*, *593*, 125622.
McColl, K. A., et al. (2017), The global distribution and dynamics of surface soil moisture, *Nature Geoscience*, *10*(2), 100-104.
Oladipo, E., and F. Hare (1986), Persistence of anomalous moisture conditions in the interior plains of North America, *Journal of climatology*, *6*(5), 485-494.
Orth, R., and S. I. Seneviratne (2013), Propagation of soil moisture memory to streamflow and evapotranspiration in Europe, *Hydrology and Earth System Sciences*, *17*(10), 3895-3911.
Pagano, M., and K. T. Halvorsen (1981), An algorithm for finding the exact significance levels of r× c contingency tables, *Journal of the American statistical Association*, *76*(376), 931-934.
Riley, M. A., et al. (2012), A tutorial introduction to adaptive fractal analysis, *Frontiers in physiology*, *3*, 371.
Shen, S., et al. (2018), Persistence and Corresponding Time Scales of Soil Moisture Dynamics During Summer in the Babao River Basin, Northwest China, *Journal of Geophysical Research: Atmospheres*, *123*(17), 8936-8948.
Song, Y. M., et al. (2019), Soil Moisture Memory and Its Effect on the Surface Water and Heat Fluxes on Seasonal and Interannual Time Scales, *Journal of Geophysical Research-Atmospheres*, *124*(20), 10730-10741.
Stahle, D. W., and M. K. Cleaveland (1988), Texas drought history reconstructed and analyzed from 1698 to 1980, *Journal of Climate*, *1*(1), 59-74.