

A Geostatistical Approach to Upscale Soil Moisture With Unequal Precision Observations

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Abstract—Upscaling ground-based moisture observations to satellite footprint-scale estimates is an important problem in remote sensing soil-moisture product validation. The reliability of validation is sensitive to the quality of input observation data and the upscaling strategy. This letter proposes a model-based geostatistical approach to scale up soil moisture with observations of unequal precision. It incorporates unequal precision in the spatial covariance structure and uses Monte Carlo simulation in combination with a block kriging (BK) upscaling strategy. The approach is illustrated with a real-world application for upscaling soil moisture in the Heihe Watershed Allied Telemetry Experimental Research experiment. The results show that BK with unequal precision observations can consider both random ground-based measurement errors and upscaling model error to achieve more reliable estimates. We conclude that this approach is appropriate to quantify upscaling uncertainties and to investigate the error propagation process in soil-moisture upscaling.

Index Terms—Block kriging (BK), Heihe Watershed Allied Telemetry Experimental Research (HiWATER), Monte Carlo simulation, remote sensing product validation.

I. INTRODUCTION

SOIL moisture is a key variable in controlling the exchange of heat and water energy between the atmosphere and land surface [1]. It is important in agricultural and irrigation management practices, particularly in semiarid and arid regions. In practice, there are two categories of soil-moisture estimation methods [2]: one makes use of remote sensing data, and the other uses *in situ* measurements. Remotely sensed measurements of soil moisture can be obtained from passive microwave radiometers, scatterometers, and synthetic aperture radars and using thermal methods. A series of global-scale remotely sensed surface soil-moisture products has been available for several decades [3]. Compared with *in situ* measurements, remote sensing provides the capability to obtain spatially exhaustive observations of surface soil moisture at global and regional scales. However, the spatiotemporal resolution and accuracy

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may not meet those required for specific applications. The validation of satellite-based soil-moisture products is important to provide users with an assessment of their accuracy and reliability. *In situ* soil-moisture measurements, particularly emerging wireless sensor network (WSN) technologies, provide dynamic real-time soil-moisture observations [4]. These observations could be used for the improved characterization of hydrological fluxes, calibration and validation of remote sensing data, and development of upscaling and downscaling techniques [5].

A number of studies have been conducted to validate the performance of remotely sensed soil-moisture products, using *in situ* measurements [6], [7]. These studies concur that a significant challenge in validation is the disparity in spatial scales between satellite retrievals and *in situ* observations [8]. The conventional solution is to take the arithmetic mean of multiple ground-based observations to obtain satellite footprint-scale estimates and make a comparison with the corresponding satellite soil-moisture product. The comparison is based on the assumption that ground measurements are more accurate than the remote sensing retrievals and that the upscaled estimates represent the *true* value of footprint-scale soil moisture [9]. However, extensive observations at small scale ($\sim 100 \text{ km}^2$) suggest that upscaling via simple averaging of soil-moisture data from randomly distributed measurement sites results in unacceptable upscaling errors, unless high sampling densities are maintained. If such high spatial densities are unavailable in practice, more sophisticated upscaling strategies are required.

The upscaling of soil water processes is one of the critical issues in soil process research [10], [11]. Current data sets that provide sufficient information to extensively validate existing upscaling approaches are lacking [1]. The Heihe Watershed Allied Telemetry Experimental Research (HiWATER) [12] is a comprehensive ecohydrological experiment that uses a flux observing matrix and an ecohydrological WSN to promote interdisciplinary watershed-scale scientific research. One objective of HiWATER is to design *in situ* sampling strategies and develop upscaling techniques for remote sensing validation [13]. For these purposes, three kinds of soil-moisture WSNs with different measurement precision have been deployed to continuously observe soil moisture in an irrigation district area (see [12, Fig. 4]). Using data sets gleaned from WSNs, a crucial issue is how to scale up soil moisture with unequal precision observations to validate an instantaneous pixel-scale average with sufficient accuracy.

A number of upscaling strategies have been developed to reduce the detrimental impact of spatial sampling errors on the reliability of satellite product validation [8]. For example, the issue of scaling in the field of microwave radiometric remote

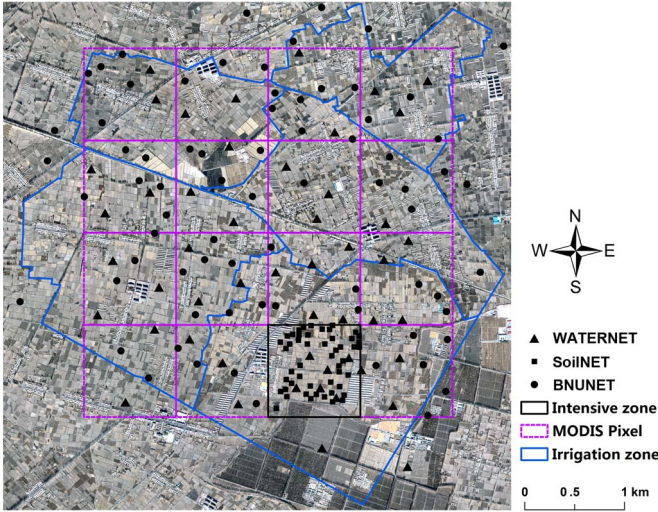


Fig. 1. Soil-moisture monitoring network design in the Yingke-Daman irrigation district. The background is a high-resolution remote sensing image.

sensing has been investigated by Liou *et al.* [14], [15], who examined and addressed the effect of scaling on the interpretability of mixed pixel radiobrightness. However, little to no research addresses the issue of random measurement errors in upscaling soil moisture. Therefore, this letter proposes a model-based geostatistical [16] approach to scale up soil moisture with consideration of unequal precision observations, by combining block kriging (BK) with an uncertain spatial covariance structure. The proposed upscaling strategy can improve soil-moisture estimation because it considers not only soil-moisture spatial variability but also its measurement errors. The objective is to improve the reliability of satellite soil-moisture product validation as used in HiWATER.

II. MATERIALS AND METHODS

A. Study Area and Data Description

The area of interest is the Yingke-Daman irrigation district, which is in an artificial oasis-riparian ecosystem-wetland-desert compound in the middle reaches of the Heihe River Basin, China [12]. It is one of the main study areas of HiWATER. The district covers $38^{\circ}50' - 38^{\circ}54'N$ and $100^{\circ}19' - 100^{\circ}24'E$ (see Fig. 1) and is in a typical semiarid and arid agricultural region with maize, wheat, and vegetables as major crops. Precipitation is approximately 100–250 mm per year, while potential evaporation is about 1200–1800 mm per year. Agricultural irrigation is essential for crop growth.

To acquire soil-moisture information in HiWATER, three types of new ecohydrological WSNs (i.e., WATERNET, SoilNET, and BNUNET), with varying measurement precision, were designed and deployed to monitor surface soil moisture (~ 5 cm depth) [13]. The spatial distribution of the nodes is shown in Fig. 1, which covers approximately 16 (4×4) Moderate-Resolution Imaging Spectroradiometer (MODIS) 1-km spatial resolution pixels. One MODIS pixel (black square in Fig. 1) covers 50 SoilNET nodes and was designed as an intensive observation zone to capture small-scale soil-moisture variation. Details on the properties of WSNs are given in

TABLE I
PROPERTIES OF THREE KINDS OF WSN

Type	Soil moisture Sensor	Number	Instrument error (s.e.)
WATERNET	Hydra Probe II	50	$0.010 \text{ m}^3 \text{ m}^{-3}$
SoilNET	Simple soil moisture probe	50	$0.015 \text{ m}^3 \text{ m}^{-3}$
BNUNET	Beijing Normal University sensor	80	$0.020 \text{ m}^3 \text{ m}^{-3}$

Table I. The magnitude of instrument errors for each type of WSN was determined by laboratory calibration [17].

B. Soil-Moisture Upscaling Strategies

Assume that vector \mathbf{Z} contains N point-scale soil-moisture measurements within a given remotely sensed footprint v . Then, the footprint-scale soil moisture may be estimated via the upscaling function f_{up} as $Z_{\text{up}}(v) = f_{\text{up}}(\mathbf{Z})$. Uncertainties in $Z_{\text{up}}(v)$ can arise from three separate sources [8], i.e., random instrument measurement error impacting the elements of \mathbf{Z} , sampling error due to a representation of the footprint by a finite set of points, and upscaling error from lack of knowledge concerning the appropriate function for f_{up} . We aimed to combine both measurement error and upscaling error in the following upscaling approach.

BK With Unequal Precision Observations: The simplest way to scale up a set of sparse ground-based soil-moisture measurements is to define f_{up} as a simple linear average, i.e., $\hat{Z}_{\text{up}}(v) = f_{\text{up}}(\mathbf{Z}) = N^{-1} \sum_{i=1}^N Z_i$. Here, all point measurements are given equal weight. This would be optimal if the observation locations had been selected using simple random sampling, in which case a design-based upscaling technique can be used, but a model-based approach must be used in case of convenience sampling [18]. In such case, unweighed averaging is suboptimal if soil moisture is spatially autocorrelated, and BK [19] can be used to derive optimal weights w_i for each observation and thereby improve estimates of $Z_{\text{up}}(v)$ by $\hat{Z}_{\text{up}}(v) = \sum_{i=1}^N w_i Z_i$.

In the case of soil moisture with m types of unequal precision observations, the block value $Z_{\text{up}}(v)$ can be estimated as a linear combination of observations as follows:

$$\hat{Z}_{\text{up}}(v) = \sum_{i=1}^{n_1} w_i^1 Z_i^1 + \sum_{i=1}^{n_2} w_i^2 Z_i^2 + \dots + \sum_{i=1}^{n_m} w_i^m Z_i^m = \mathbf{W}\mathbf{Z} \quad (1)$$

where $n_1 + n_2 + \dots + n_m = N$. $\mathbf{Z} = [Z^1, Z^2, \dots, Z^m]$ is a $1 \times N$ vector of point observations and $\mathbf{W} = [w^1, w^2, \dots, w^m]'$ is an $N \times 1$ vector of BK weights. The \hat{Z}_{up} must be unbiased and minimize the error variance $\sigma_{\text{up}}^2 = \text{Var}\{\hat{Z}_{\text{up}} - Z_{\text{up}}\}$.

The BK system is written as follows [20]:

$$\begin{cases} \mathbf{C}\mathbf{W} - \mu\mathbf{1} = \mathbf{c}_v \\ \mathbf{W}'\mathbf{1} = 1 \end{cases} \quad (2)$$

where $\mathbf{1}$ is an N -dimensional row vector whose elements are set to unity, \mathbf{C} is the variance-covariance matrix of the soil-moisture ground observations, and \mathbf{c}_v is the vector of covariances between the soil-moisture ground observations and that of the remotely sensed footprint v . \mathbf{C} and \mathbf{c}_v are derived from the variogram [21].

From (2), the BK estimator and the corresponding estimation error variance can be obtained as

$$\hat{Z}_{\text{up}}(v) \equiv \mathbf{WZ} = \{\mathbf{c}_v + \mathbf{1d}/(\mathbf{1}'\mathbf{C}^{-1}\mathbf{1})\}'\mathbf{C}^{-1}\mathbf{Z} \quad (3)$$

$$\sigma_{\text{up}}^2(v) = c(v) - \mathbf{c}_v'\mathbf{C}^{-1}\mathbf{c}_v + \mathbf{d}'(\mathbf{1}'\mathbf{C}^{-1}\mathbf{1})^{-1}\mathbf{d} \quad (4)$$

where $\mathbf{d} = \mathbf{1} - \mathbf{1}'\mathbf{C}^{-1}\mathbf{c}_v$ and $c(v)$ is the within-block covariance, which is approximated by the arithmetic average of the covariances defined between any discretizing points in block v [19].

It is assumed that instrument errors for each type of WSN follow a $N(0, \sigma^m)$ Gaussian normal distribution after instrument intercalibration [22]. σ^m represents the instrument standard error. As listed in Table I, the instrument standard errors vary with WSN. If observations without consideration of measurement errors are used, the estimation in soil-moisture upscaling with (3) will be biased, due to the erroneous estimation of the variance-covariance matrix or variogram [16], [23]. The corresponding prediction error variance in (4) will also be biased.

With respect to the variable measurement errors of each WSN type, \mathbf{C} and \mathbf{c}_v in (2)–(4) can be decomposed as

$$\mathbf{C} = \begin{bmatrix} C^{11} & C^{12} & \dots & C^{1m} \\ C^{21} & C^{22} & \dots & C^{2m} \\ \vdots & \vdots & \ddots & \vdots \\ C^{m1} & C^{m2} & \dots & C^{mm} \end{bmatrix}, \quad \mathbf{c}_v = [c_v^1, c_v^2, \dots, c_v^m]^T \quad (5)$$

where diagonal items of \mathbf{C} are derived from the covariance function of one type of WSN. Off-diagonal items represent the cross-covariance function between two WSN types.

To implement \mathbf{C} and \mathbf{c}_v calculation with unequal precision observations, a Monte Carlo simulation approach is used. First, the magnitude of instrument errors is controlled by adjusting the value of σ^m . With the assumption that the instrument errors for each WSN type follow an $N(0, \sigma^m)$ distribution, error-perturbed observations can be obtained by adding random instrument errors to the original observations. Next, \mathbf{C} and \mathbf{c}_v can be calculated by (5) with these error-perturbed observations. Consequently, a number of realizations of $\hat{Z}_{\text{up}}(v)$ and $\sigma_{\text{up}}^2(v)$ estimates by Monte Carlo simulation are obtained. The mean value of these realizations of $\hat{Z}_{\text{up}}(v)$ and $\sigma_{\text{up}}^2(v)$ represents the upscaling soil-moisture estimation and corresponding estimation error variance, respectively.

III. RESULTS

The upscaling strategy for soil moisture with unequal precision observations is based on the BK procedure described earlier. First, 28 days of soil-moisture observations (July 9–August 5, 2012) were obtained from the HiWATER website (<http://hiwater.westgis.ac.cn>) [17]. For remote sensing product validation, we only considered soil-moisture observations during satellite and aircraft flyovers.

To model the spatial variability of soil moisture, variograms were calculated, and appropriate variogram models were fitted. Taking observations on July 24, 2012 as an example, the variograms of soil moisture for all observations are shown in Fig. 2.

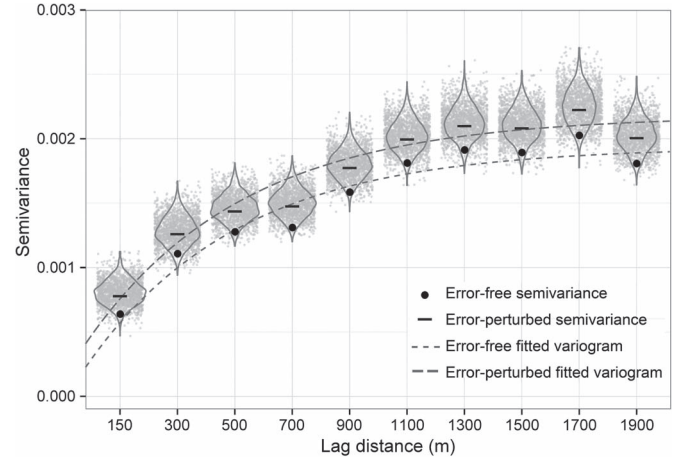


Fig. 2. Soil-moisture variogram for all observations on July 24, 2012, including two cases: One in which observations were error free and another in which they contained random instrument errors.

This includes two cases, one in which observations are taken as they are and the others in which random instrument errors were included (error-perturbed). Based on the error-perturbed soil-moisture observations, 5000 realizations of variograms were calculated using Monte Carlo simulation. Each corresponding sample variogram is shown using gray dots in Fig. 2. The short horizontal line indicates the mean value of all realizations for each lag distance. Taking mean values of all realizations as the average variability for each lag, the error-perturbed variogram was fitted by an exponential model. Fig. 2 shows that the error-perturbed variogram has a larger nugget and sill value than the error-free variogram. This result indicates that random instrument error has a significant impact on the spatial variability of soil moisture.

To implement the variance-covariance matrix in (5), we calculated the variogram within each WSN type and the cross-variogram between two types. The results are shown in Fig. 3. The left panel shows variograms obtained separately from the three WSN types. Black dots and short horizontal lines represent semivariance calculated from the error-free and simulated error-perturbed observations, respectively. Due to instrument error in WATERNET, SoilNET, and BNUNET, the nugget and sill increased by an average of 0.01^2 , 0.015^2 , and 0.02^2 semivariance for each lag. The same phenomenon appeared in the cross-variogram.

For comparison, three upscaling strategies, simple average, BK without considering instrument error (error-free BK), and BK with unequal precision observations (error-perturbed BK), were adopted to upscale soil moisture within the 4×4 MODIS footprint. The time series of soil-moisture estimates and corresponding estimation error standard deviation (SD) are shown in Figs. 4 and 5, respectively. As shown in Fig. 4, the estimation of soil moisture does not show a significant difference among these three upscaling strategies. Time series averages for simple average, error-free BK, and error-perturbed BK soil-moisture estimates are $0.267 \text{ m}^3 \text{ m}^{-3}$, $0.264 \text{ m}^3 \text{ m}^{-3}$, and $0.260 \text{ m}^3 \text{ m}^{-3}$, respectively. The comparison indicates that soil-moisture upscaling with unequal precision measurement potentially causes 1.5% smaller estimates than error-free BK estimation.

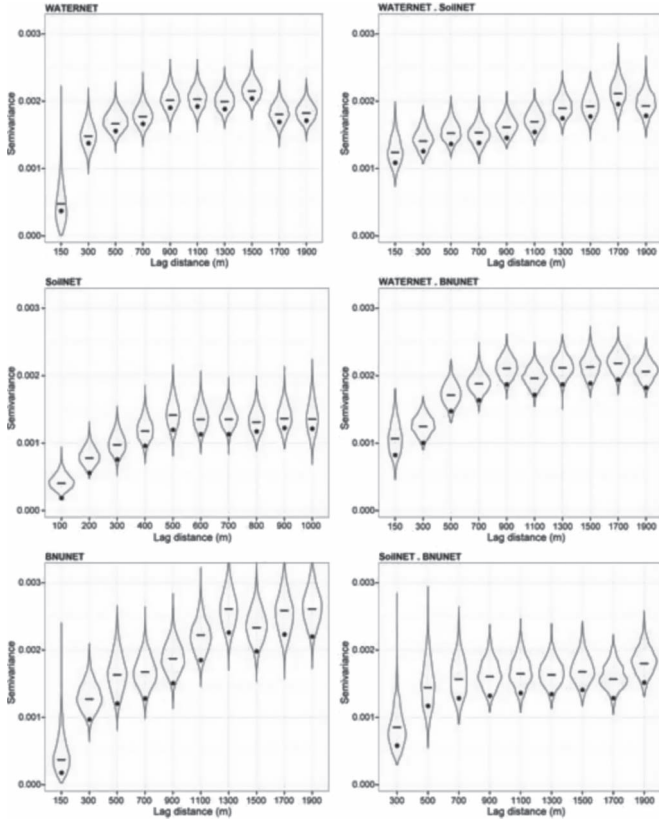


Fig. 3. Variogram of soil moisture with unequal precision observations on July 24, 2012. Variograms in left panel were calculated within each WSN type, whereas those in the right panels were calculated between two WSN types.

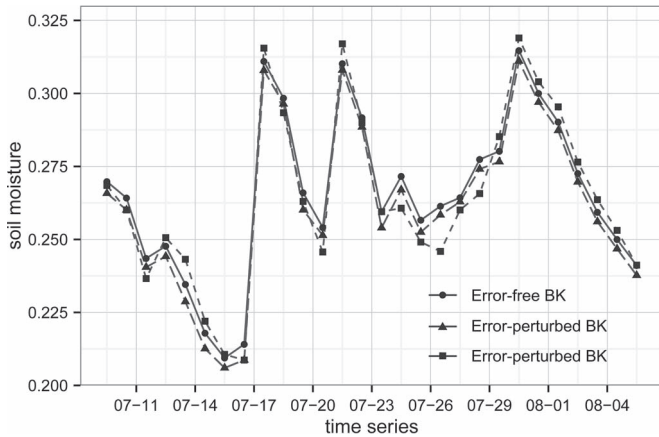


Fig. 4. Soil-moisture estimation using simple average of observations, BK with error-free observations, and BK with unequal precision observations.

The time series of estimation error SD (see Fig. 5) clearly indicates that error-free BK and error-perturbed BK significantly reduce estimation error SD, more than the simple average method. The reason is that BK takes soil-moisture spatial autocorrelation into account to provide the best linear unbiased estimation (BLUE) [19]. However, BLUE is based on the assumption that all observations are error free or have the same random measurement errors. When observations contain unequal precision instrument error, this should be accounted for in the kriging. That is why BK with unequal precision observations produces an average of 0.006 larger estimation error SD than the BK without consideration of measurement error.

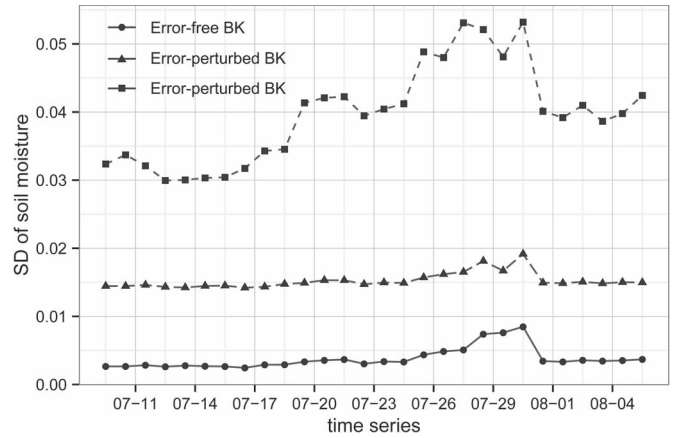


Fig. 5. Soil-moisture estimation error SD using simple average of observations, BK with error-free observations, and BK with unequal precision observations.

IV. DISCUSSION

Unequal precision observations are common practice for a range of gauging conditions, such as observers, instruments, observing periods, etc. It is important to take the accuracy of observations into account when these observations are used to estimate the block average. Standard kriging assumes that the random measurement error is the same for all observations, and when it is not, we have to take it into account [20]. To solve this problem, we present a simulation approach to scale up soil moisture with unequal precision observations. The main purpose of this letter is to investigate the measurement error propagation in soil-moisture upscaling. This approach assumes that the original observations are error free before adding random measurement errors on them, which is a strong assumption. This assumption should be checked more carefully in the future work and alternative approach such as adjusting the diagonal of the variance-covariance matrix in (5) by taking the measurement error variance as part of the variogram nugget may also be considered. Different from simulation approach, Christensen [23] developed a new heterogeneous variance measurement-error-filtered kriging (HKF) predictor in a more theoretical way for spatial prediction in the presence of measurement error. We noted that HKF could also be expanded into the BK predictor and can be used to upscale soil moisture with unequal precision observations later.

In soil-moisture upscaling, the uncertainty is commonly quantified by the estimation error variance [8]. This variance is an overall description of estimation errors, resulting from a spatial covariance function or variogram of physical quantities. Hence, what matters most is calculating the (cross-)covariance function of unequal precision observations. Multivariable geo-statistics provides a way to estimate soil moisture using additional data from auxiliary variables or other measurement sources with cokriging [24], [25]. However, its estimation of error variances is biased when observations of unequal precision are treated as if they have identical precision [20]. The spatial structure of estimation with unequal precision data, determined by the covariance function, is different from that of identical precision data. More specifically, inner constructions of BK estimation weights are of crucial importance.

Together with the uncertainty of upscaling strategy, the experiment conducted in this letter regarded observation errors as a key consideration and combined both error issues. The experimental results demonstrate that instrument error, which directly affects soil-moisture observation precision, contributes to error propagation. The covariance function is sensitive to sample data, so proper methods must be used to make full use of the unequal precision information and reduce the precision loss. Moreover, data processing methods determine error propagation patterns in view of the combination of unequal precisions of raw data and modeling errors. Therefore, the proposed strategy works well to quantify the effects of both error propagation results.

V. CONCLUSION

Upscaling ground-based soil-moisture measurements for validation of coarse-resolution satellite soil-moisture products is important because, in this way, the accuracy of remote sensing products can be assessed. In this letter, a model-based geostatistical approach was proposed to scale up soil moisture with observations of unequal precision. The method was illustrated with a real-world application to scale up soil moisture in the HiWATER experiment. By extending the existing BK upscaling method, the proposed approach can consider both random ground-based measurement errors and upscaling model error to achieve more reliable estimation. The approach is recommended for quantifying upscaling uncertainties and investigating the error propagation process in soil-moisture upscaling.

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