

1 Estimating spatially distributed soil water content at small watershed
2 scales based on decomposition of temporal anomaly and time stability
3 analysis

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9 **Abstract**

10 Soil water content (SWC) is crucial to rainfall-runoff response at the watershed scale.
11 A model was used to decompose the spatiotemporal SWC into a time-stable pattern
12 (i.e., temporal mean), a space-invariant temporal anomaly, and a space-variant
13 temporal anomaly. The space-variant temporal anomaly was further decomposed
14 using the empirical orthogonal function (EOF) for estimating spatially distributed
15 SWC. This model was compared to a previous model that decomposes the
16 spatiotemporal SWC into a spatial mean and a spatial anomaly, with the latter being
17 further decomposed using the EOF. These two models are termed temporal anomaly
18 (TA) model and spatial anomaly (SA) model, respectively. We aimed to test the
19 hypothesis that underlying (i.e., time-invariant) spatial patterns exist in the
20 space-variant temporal anomaly at the small watershed scale, and to examine the
21 advantages of the TA model over the SA model in terms of the estimation of spatially

22 distributed SWC. For this purpose, a dataset of near surface (0–0.2 m) and root zone
23 (0–1.0 m) SWC, at a small watershed scale in the Canadian prairies, was analyzed.
24 Results showed that underlying spatial patterns exist in the space-variant temporal
25 anomaly because of the permanent controls of “static” factors such as depth to the
26 CaCO₃ layer and organic carbon content. Combined with time stability analysis, the
27 TA model improved the estimation of spatially distributed SWC over the SA model,
28 especially for dry conditions. Further application of these two models demonstrated
29 that the TA model outperformed the SA model at a hillslope in the Chinese Loess
30 Plateau, but the performance of these two models in the GENCAI network (~250 km²)
31 in Italy was equivalent. The TA model can be used to construct a high-resolution
32 distribution of SWC at small watershed scales from coarse-resolution remotely sensed
33 SWC product.

34 Keywords: Soil moisture; Soil water downscaling; Empirical orthogonal function;
35 Statistical models; Time stability

36 **1. Introduction**

37 Soil water content (SWC) of surface soils exerts a major influence on a series of
38 hydrological processes such as runoff and infiltration (Famiglietti et al., 1998;
39 Vereecken et al., 2007; She et al., 2013a). Soil water content in the root zone is, in
40 many cases, linked to vegetative growth (Wang et al., 2012; Ward et al., 2012; Jia and
41 Shao, 2013). Obtaining accurate information on the spatiotemporal SWC is crucial for
42 improving hydrological prediction and soil water management (Venkatesh et al., 2011;

43 Champagne et al., 2012; She et al., 2013b; Zhao et al., 2013). While remote sensing
44 has advanced SWC measurements of surface soils (<5 cm in depth) at basin
45 (2,500–25,000 km²) and continental scales (Robinson et al., 2008), characterization of
46 spatially distributed SWC at small watershed (0.1–80 km²) scales still poses a
47 challenge. A method is needed for estimating spatially distributed SWC in the near
48 surface and root zone at watershed scales.

49 Time stability of SWC, which refers to similar spatial patterns of SWC across
50 different measurement times (Vachaud et al., 1985; Brocca et al., 2009), has been used
51 for estimating spatially distributed SWC (Starr, 2005; Perry and Niemann, 2007;
52 Blöschl et al., 2009). This method is conceptually-appealing, but assumes completely
53 time-stable spatial patterns of SWC.

54 The time-stable pattern does not explain all of the spatial variances in SWC,
55 indicating the existence of time-variant components (Starr, 2005). In order to identify
56 underlying patterns of SWC that have time-variant components, the spatiotemporal
57 SWC was decomposed into a spatial mean and a spatial anomaly. The spatial anomaly
58 of the SWC was further decomposed into the sum of the product of time-invariant
59 spatial patterns (EOFs) and temporally varying, but spatially constant coefficients
60 (ECs) using the empirical orthogonal function (EOF) (Fig. 1) (Jawson and Niemann,
61 2007; Perry and Niemann, 2007, 2008; Joshi and Mohanty, 2010; Korres et al., 2010;
62 Busch et al., 2012). Spatially distributed SWC estimates based on the decomposition
63 of spatial anomaly outperformed those based on time-stable patterns (Perry and
64 Niemann, 2007).

65 Recently, the spatiotemporal SWC was also decomposed into a temporal mean and
66 a temporal anomaly (Mittelbach and Seneviratne, 2012) (Fig. 1). Previous studies
67 indicated that the contribution of the temporal anomaly to the total spatial variance
68 was notable (Mittelbach and Seneviratne, 2012; Brocca et al., 2014; Rötzer et al.,
69 2015). These studies, however, only focused on surface soils at large scales (> 250
70 km^2). Vanderlinden et al. (2012) suggested that the temporal mean may be further
71 decomposed into its spatial mean and residuals, and the temporal anomaly may be
72 further decomposed into space-invariant term (i.e., spatial mean of temporal anomaly)
73 and space-variant term (i.e., spatial residuals of temporal anomaly) (Fig. 1). Note that
74 the spatial variance in the temporal anomaly (Mittelbach and Seneviratne, 2012)
75 equals that of the space-variant term of the temporal anomaly (Vanderlinden et al.,
76 2012). The further decomposition of the temporal anomaly may be physically
77 meaningful, because the space-invariant and space-variant terms in the temporal
78 anomaly may be forced differently. However, the models of Mittelbach and
79 Seneviratne (2012) and Vanderlinden et al. (2012) have not been used for estimating
80 spatially distributed SWC. If the space-variant terms are ignored during the estimation
81 of spatially distributed SWC, their models are equivalent to that based on time-stable
82 patterns. Therefore, estimation of spatially distributed SWC may be improved by
83 incorporating the space-variant term of the temporal anomaly if underlying (i.e.,
84 time-invariant) spatial patterns exist in the temporal anomaly.

85 To our knowledge, the importance of the space-variant term of the temporal
86 anomaly and its physical meaning at small watershed scales is not well-known. Based

87 on previous studies (Perry and Niemann, 2007; Mittelbach and Seneviratne, 2012;
88 Vanderlinden et al., 2012), we assume soil water dynamics at watershed scales can be
89 decomposed into three components (Fig. 1): (1) time-stable pattern (i.e., temporal
90 mean, spatial forcing): the “static” factors such as soil and topography control the
91 pattern; (2) space-invariant temporal anomaly (temporal forcing): the “dynamic”
92 factors such as meteorological variables and vegetation change with time, and
93 therefore modify SWC in time, regardless of spatial locations; and (3) space-variant
94 temporal anomaly (interactions between spatial forcing and temporal forcing): this
95 term represents interactions between “static” and “dynamic” factors. For example,
96 SWC recharge introduced by a rainfall may be modified by topography through
97 runoff processes; SWC loss triggered by evapotranspiration may be regulated by
98 topography through solar radiation exposure.

99 The “static” factors may be persistent in the space-variant temporal anomaly, and
100 their impacts on the space-variant temporal anomaly likely change with time. Thus,
101 we hypothesize that some underlying (i.e., time-invariant) spatial patterns exist in the
102 space-variant temporal anomaly, and their impacts can be modulated by a time
103 coefficient, both of which can be obtained by the EOF method (Fig. 1). If the
104 hypothesis is true, the estimation of spatially distributed SWC utilizing the EOF
105 decomposition may outperform the one suggested by Perry and Niemann (2007). This
106 is because: (1) the spatial anomaly which was decomposed using the EOF in Perry
107 and Niemann (2007) lumped the time-stable pattern and space-variant temporal
108 anomaly together (Fig. 1); (2) the underlying spatial patterns in the spatial anomaly

109 may not fully capture both time-stable patterns and patterns in the space-variant
110 temporal anomaly due to the possible nonlinear relations between these two terms.

111 Therefore, the objectives were (1) to test the hypothesis that underlying spatial
112 patterns exist in the space-variant temporal anomaly at small watershed scales and (2)
113 to examine whether the decomposition of the space-variant temporal anomaly using
114 the EOF has any advantages over the decomposition of the spatial anomaly (Perry and
115 Niemann, 2007) for estimating spatially distributed SWC. Two steps were included in
116 the estimation of spatially distributed SWC. First, the spatial mean SWC was upscaled
117 from the SWC measurement at the most time-stable location using time stability
118 analysis. Following this, the spatially distributed SWC was downscaled from the
119 estimated spatial mean SWC. For the purpose of this study, spatiotemporal SWC
120 datasets at depths of near surface (0–0.2 m) and root zone (0–1.0 m) from a Canadian
121 prairie landscape were used. Spatiotemporal SWC of samples taken 0–0.06 m from a
122 hillslope (100 m) in the Chinese Loess Plateau and 0–0.15 m from the GENCAI
123 network (~250 km²) in Italy were also used to further demonstrate conditions under
124 which the decomposition of the spatial anomaly was beneficial to the estimation of
125 spatially distributed SWC.

126 **2. Materials and methods**

127 2.1 Study area and data collection This study was mainly conducted in the Canadian
128 prairie pothole region (hereafter abbreviated as Canadian site) at St. Denis National
129 Wildlife Area (52°12' N, 106°50' W) with an area of 3.6 km². This area has a humid

130 continental climate (Peel et al., 2007), and had a mean annual air temperature of
131 1.9 °C and a mean annual precipitation of 402 mm during the study period (Fig. 2). A
132 variety of depressions, knolls, and knobs result in a sequence of undulating slopes
133 (Biswas et al., 2011). The elevation varies from 554.8 to 557.5 m. The soils are
134 dominated by clay loam textured Mollisols (Soil Survey Staff, 2010) and covered by
135 mixed grass, i.e., smooth brome grass (*Bromus inermis*) and alfalfa (*Medicago sativa*
136 L.). The near surface soil porosity ranges from 38% (knolls) to 70% (depressions).
137 Calcium carbonates (CaCO_3) derived mostly from fragments of limestone rocks are
138 common in the Canadian Prairies. The CaCO_3 is dissolved by the slightly acidic
139 rainwater moving through the upper horizons and deposited to lower horizons. The
140 heterogeneous amount of infiltrated water resulted in a varying depth of CaCO_3 layer
141 ranging from almost 0 m in the knolls to 2.1 m in the depressions. A 576 m long
142 sampling transect with 128 sampling locations spaced at 4.5 m intervals was
143 established over several rounded knolls and depressions. At each location, a time
144 domain reflectometry probe was used to measure SWC of the near surface soil (0–0.2
145 m), and a neutron probe was used to collect SWC measurements at 0.2 m intervals
146 between a depth of 0.2 and 1.0 m. The SWC was measured on a volumetric basis and
147 expressed as a percentage (%) volume of water per unit soil volume. The SWC of the
148 root zone was calculated by averaging the SWC of 0–0.2, 0.2–0.4, 0.4–0.6, 0.6–0.8,
149 and 0.8–1.0 m. Soil water content was measured on 23 dates from July 17, 2007 to
150 September 29, 2011. The SWC dataset was collected in all seasons except winter, and
151 accurately portrays the variations in soil water conditions in the study area. In addition

152 to the SWC dataset, the soil, vegetative, and topographical properties were obtained at
153 each sampling location. These properties included soil particle components (clay, silt,
154 and sand contents), bulk density, soil organic carbon (SOC) content for the surface
155 layer, A horizon depth, C horizon depth, depth to the CaCO₃ layer, leaf area index,
156 elevation, cos(aspect), slope, curvature, gradient, upslope length, solar radiation,
157 specific contributing area, convergence index, wetness index, and flow connectivity.
158 Detailed information on the measurements can be found in Biswas et al. (2012). The
159 datasets from the Canadian site were used to demonstrate the following two aspects in
160 detail: (1) different components of spatiotemporal SWC and their contributing factors,
161 and (2) the advantages of the new decomposition method over the method suggested
162 by Perry and Niemann (2007) in terms of the estimation of spatially distributed SWC.

163 Besides the Canadian site, datasets from a hillslope scale in a Chinese site and a
164 large watershed scale in a Italian site were applied. Along a hillslope of 100 m in
165 length in the Chinese Loess Plateau, SWC of 0–0.06 m was measured 136 times from
166 June 25, 2007 to August 30, 2008 by a Delta-T Devices Theta probe (ML2x) at 51
167 locations (Hu et al., 2011). The hillslope was covered by *Stipa bungeana* Trin. and
168 *Medicago sativa* L. in sandy loam and silt loam soils. In the GENCAI network (~250
169 km²) in Italy, SWC of 0–0.15 m was measured by a TDR probe at 46 locations, 34
170 times from February to December in 2009 (Brocca et al., 2012, 2013). The GENCAI
171 area was dominated by grassland with a flat topography, in silty clay soils. With these
172 two datasets, spatially distributed SWC was estimated using the two different
173 decomposition methods. Performances in estimation of spatially distributed SWC

174 were compared among all three sites to further demonstrate conditions under which
175 the new decomposition outperformed the method suggested by Perry and Niemann
176 (2007).

177 **2.2 Statistical models for decomposing soil water content**

178 Spatiotemporal SWC at small watershed scales was decomposed into three
179 components: time-stable pattern, space-invariant temporal anomaly, and space-variant
180 temporal anomaly. This model was compared to the one that decomposed SWC into
181 spatial mean and spatial anomaly (Perry and Niemann, 2007). Both the space-variant
182 temporal anomaly and spatial anomaly were decomposed using the EOF method. The
183 two models are termed temporal anomaly (TA) model and spatial anomaly (SA)
184 model, respectively. Figure 1 displays the differences between the two models. Each
185 component will be explained in detail later. The explanation of nomenclatures is listed
186 in Table A1. Because we focus on estimating spatial distribution of SWC at any given
187 time, only spatial variances of SWC were taken into account. Therefore, the variance
188 or covariance denotes the quantity in space without specifications.

189 **2.2.1 The SA model**

190 Perry and Niemann (2007) expressed SWC at location n and time t (S_{tn}) as (Fig.
191 1):

$$192 \quad S_{tn} = S_{t\hat{n}} + Z_{tn}, \quad (1)$$

193 where $S_{t\hat{n}}$ is the spatial mean SWC at time t (temporal forcing) and Z_{tn} is the
194 spatial anomaly of SWC (lumped spatial forcing and interactions). The subscript \hat{n}
195 (\hat{t}) indicates a space (time) averaged quantity.

196 According to Perry and Niemann (2007), $S_{t\hat{n}}$ can be estimated by remote sensing,

197 water balance models, and in situ soil water measurement at a representative (or
 198 time-stable) location. The in situ soil water measurement method was selected
 199 because the representative location can be easily determined with prior SWC datasets.
 200 By measuring SWC only at the most time-stable location (s) and future time t (S_{ts}),
 201 $S_{\hat{m}}$ can be estimated using (Grayson and Western, 1998):

$$202 \quad S_{\hat{m}} = \frac{S_{ts}}{1 + \delta_{ts}} \quad , \quad (2)$$

203 where the s was identified using the time stability index of mean absolute bias error
 204 (Hu et al., 2010, 2012). The δ_{ts} is the temporal mean relative difference of SWC at
 205 the s , which was calculated with prior measurements.

206 Spatial anomaly (Z_m) can be reconstructed by the sum of the product of
 207 time-invariant spatial structures (EOFs) and temporally varying coefficients (ECs)
 208 using the EOF method (Perry and Niemann, 2007; Joshi and Mohanty, 2010;
 209 Vanderlinden et al., 2012). The ECs correspond to the eigenvectors of the matrix of
 210 spatial covariance of the Z_m , and the EOFs are obtained by projecting the Z_m onto
 211 the matrix ECs as: EOFs = Z_m ECs. The number of EOF (or EC) series equals the
 212 number of sampling dates. Each EOF series corresponds to one value at each location,
 213 and each EC series has one value at each measurement time. Each EOF is chosen to
 214 be orthogonal to other EOFs, and the lower-order EOFs account for as much variance
 215 as possible. The sum of variances of all EOFs equals the sum of variances of Z_m
 216 from all measurement times.

217 Usually, a substantial amount of variance can be explained by a small number of
 218 EOFs. Johnson and Wichern (2002) suggested the eigenvalue confidence limits

219 method for selecting the number of EOFs. Once the number of significant EOFs at a
 220 confidence level of 95% is selected, Z_{tm} can be estimated as the sum of the product
 221 of significant EOFs and associated ECs as:

$$222 \quad Z_{tm} = \sum \text{EOF}^{\text{sig}} \times (\text{EC}^{\text{sig}})^T, \quad (3)$$

223 where EOF^{sig} represents the significant EOFs of the Z_{tm} obtained during model
 224 development, EC^{sig} is the associated temporally varying coefficient, and the
 225 superscript T represents matrix transpose. Following Perry and Niemann (2007), the
 226 associated significant EC at time t (EC_t), is estimated by the cosine relationship
 227 between EC and $S_{\hat{m}}$ developed using prior measurements:

$$228 \quad \text{EC}_t = a + b \cos\left(\frac{2\pi}{c} S_{\hat{m}} - d\right), \quad (4)$$

229 where a , b , c , and d are the fitted parameters using prior measurements and $S_{\hat{m}}$ is
 230 estimated from Eq. (2). By using the continuous function, EC_t can be estimated at
 231 any $S_{\hat{m}}$ values, which allows for the estimation of spatially distributed SWC at any
 232 soil water conditions.

233 **2.2.2 The TA model**

234 Mittelbach and Seneviratne (2012) decomposed the S_{tm} into a time-stable pattern
 235 (i.e., temporal mean) and a temporal anomaly component (Fig. 1):

$$236 \quad S_{tm} = M_{\hat{m}} + A_{tm}, \quad (5)$$

237 where $M_{\hat{m}}$ is the time-stable pattern (spatial forcing) controlled by “static” factors
 238 such as soil properties and topography; A_{tm} refers to the temporal anomaly (lumped
 239 temporal forcing and interactions). The variance of SWC ($\sigma_{\hat{n}}^2(S_{tm})$) is the sum of
 240 variance of the $M_{\hat{m}}$ ($\sigma_{\hat{n}}^2(M_{\hat{m}})$), variance of the A_{tm} ($\sigma_{\hat{n}}^2(A_{tm})$), and two times of

241 covariance between $M_{\hat{m}}$ and A_m ($2\text{cov}(M_{\hat{m}}, A_m)$), which can be expressed as:

$$242 \quad \sigma_{\hat{n}}^2(S_m) = \sigma_{\hat{n}}^2(M_{\hat{m}}) + 2\text{cov}(M_{\hat{m}}, A_m) + \sigma_{\hat{n}}^2(A_m). \quad (6)$$

243 Because the A_m in Mittelbach and Seneviratne (2012) is a lumped term, it can be
 244 further decomposed into space-invariant temporal anomaly ($A_{\hat{m}}$, i.e., temporal
 245 forcing) and space-variant temporal anomaly (R_m , i.e., interactions) (Vanderlinden et
 246 al., 2012). At a watershed scale, the $A_{\hat{m}}$ is controlled by temporally varying factors
 247 such as meteorological variables and vegetation. Positive and negative $A_{\hat{m}}$
 248 correspond to relatively wet and dry periods, respectively. The R_m refers to the
 249 redistribution of $A_{\hat{m}}$ among different locations due to the interactions between
 250 spatial forcing and temporal forcing. For example, soil and topography regulate how
 251 much rainfall enters soil and how much water runs off or runs on at a location. This,
 252 in turn, dictates vegetation growth in a water-limited environment. Therefore, S_m
 253 can also be expressed as (Fig. 1):

$$254 \quad S_m = M_{\hat{m}} + A_{\hat{m}} + R_m. \quad (7)$$

255 The temporal trends of $A_{\hat{m}}$ in Eq. (7) and $S_{\hat{m}}$ in Eq. (1) are the same as both
 256 represent temporal forcing. Because the $A_{\hat{m}}$ is space-invariant and orthogonal to the
 257 $M_{\hat{m}}$ and R_m in a space, $\sigma_{\hat{n}}^2(S_m)$ in Eq. (6) can also be written as:

$$258 \quad \sigma_{\hat{n}}^2(S_m) = \sigma_{\hat{n}}^2(M_{\hat{m}}) + 2\text{cov}(M_{\hat{m}}, R_m) + \sigma_{\hat{n}}^2(R_m), \quad (8)$$

259 where $\text{cov}(M_{\hat{m}}, R_m)$ is the covariance between the $M_{\hat{m}}$ and R_m , and $\sigma_{\hat{n}}^2(R_m)$ is
 260 the variance of the R_m . Apparently, $2\text{cov}(M_{\hat{m}}, R_m)$ equals $2\text{cov}(M_{\hat{m}}, A_m)$, and
 261 $\sigma_{\hat{n}}^2(R_m)$ equals $\sigma_{\hat{n}}^2(A_m)$. The percent (%) of $\sigma_{\hat{n}}^2(M_{\hat{m}})$, $2\text{cov}(M_{\hat{m}}, R_m)$, and
 262 $\sigma_{\hat{n}}^2(R_m)$ out of the $\sigma_{\hat{n}}^2(S_m)$ are calculated. The $\text{cov}(M_{\hat{m}}, R_m)$ can be negative at

263 some conditions, for example, when the depressions correspond to greater $M_{\hat{m}}$ and
 264 more negative R_{tm} values in the discharge periods. This resulted in percentage of
 265 $\sigma_{\hat{n}}^2(M_{\hat{m}})$ and $\sigma_{\hat{n}}^2(R_{tm}) > 100\%$ and percentage of $2\text{cov}(M_{\hat{m}}, R_{tm}) < 0\%$
 266 (Mittelbach and Seneviratne, 2012; Brocca et al., 2014; Rötzer et al., 2015). If R_{tm}
 267 is zero at any time or location, there are no interactions between spatial forcing and
 268 temporal forcing, $\sigma_{\hat{n}}^2(S_{tm})$ and the spatial trends of SWC are consistent over time.
 269 Therefore, R_{tm} is directly responsible for temporal change in the spatial variability
 270 of SWC.

271 If some underlying spatial patterns exist in R_{tm} , R_{tm} can be reconstructed by the
 272 sum of the product of time-invariant spatial structures (EOFs) and time-dependent
 273 coefficients (ECs) using the EOF method. Note that the number of EOF (or EC) series
 274 also equals the number of sampling dates.

275 For estimation of spatially distributed SWC, R_{tm} is estimated by the same method
 276 as Z_{tm} using Eq. (3). The $M_{\hat{m}}$ is estimated with prior measurements by:

$$277 \quad M_{\hat{m}} = \frac{1}{m} \sum_{j=1}^m S_{tm}, \quad (9)$$

278 where m is the number of previous measurement times, and $A_{\hat{m}}$ is estimated by:

$$279 \quad A_{\hat{m}} = S_{\hat{m}} - M_{\hat{m}}, \quad (10)$$

280 where $M_{\hat{m}}$ is the spatial mean of $M_{\hat{m}}$, and $S_{\hat{m}}$ is estimated from SWC
 281 measurements at the most time-stable location using Eq. (2).

282 The Pearson correlation coefficient (R) is used to explore the linear relationships
 283 between various spatial components in the two models (i.e., EOF1 of the Z_{tm} in the
 284 SA model, $M_{\hat{m}}$, and EOF1 of the R_{tm} in the TA model) and environmental factors

285 (i.e., soil, vegetative, and topographical properties). The multiple stepwise regressions
286 are conducted to determine the percentage of variations in the spatial components
287 which the controlling factors explain.

288 **2.3 Validation and performance parameter**

289 The TA model is more complicated than the SA model. In order to evaluate the two
290 models for parsimony, AICc values are calculated (Burnham and Anderson, 2002) as:

$$291 \quad AICc = 2k + n \ln(RSS / n) + 2k(k + 1) / (n - k - 1), \quad (11)$$

292 where k is the number of parameters, n is the sample size, and RSS is the residual sum
293 of squares.

294 Both cross validation and split sample validation are used to estimate SWC
295 distribution with both models. For the cross validation, an iterative removal of 1 of the
296 23 dates is made for model development, and the SWC along the transect
297 corresponding to the removed date is estimated iteratively. For the split sample
298 validation, SWC from 14 dates of the first two years (from July 17, 2007 to May 27,
299 2009) is used for model development, and the SWC distribution of 9 dates in the
300 second two years (from July 21, 2009 to September 29, 2011) is estimated.

301 The Nash-Sutcliffe coefficient of efficiency (NSCE) is used to evaluate the quality
302 of estimation of spatially distributed SWC, which is expressed as:

$$303 \quad NSCE = 1 - \frac{\sigma_{\varepsilon}^2}{\sigma_{measure}^2}, \quad (12)$$

304 where $\sigma_{measure}^2$ is the variance of measured SWC, and σ_{ε}^2 is the mean squared
305 estimation error. A larger NSCE value implies a better quality of estimation. A paired
306 samples T-test is used to test whether the NSCE values between the TA model and the

307 SA model are statistically significant at $P < 0.05$.

308 Many factors may affect the relative performance of spatially distributed SWC
309 estimation between the TA model and the SA model. First, the degree of
310 outperformance of the TA model over the SA model may depend on the amount of
311 R_{tn} variance considered in the TA model. On one hand, the two models are identical
312 if variance of R_{tn} is close to zero or there are negligible interactions between the
313 spatial and temporal components (Fig. 1). On the other hand, if no underlying spatial
314 patterns exist in the R_{tn} or the underlying spatial patterns accounted for little
315 variance of the R_{tn} , the outperformance will also be very limited. Therefore, the
316 greater the variance of R_{tn} considered in the TA model, the more likely the TA
317 model can outperform the SA model. Second, the way of EOF decomposition may
318 also affect the relative performance. In the SA model, EOF decomposition is
319 performed on lumped time-stable patterns ($M_{\hat{tn}}$) and space-variant temporal anomaly
320 (R_{tn}). In the TA model, however, EOF decomposition is made only on the R_{tn} . In
321 theory, the two models will be identical if the $M_{\hat{tn}}$ and the first underlying spatial
322 pattern (i.e., EOF1) of the R_{tn} were perfectly correlated. If a nonlinear relationship
323 exists between them, lumping the $M_{\hat{tn}}$ and R_{tn} together, as in the SA model,
324 would weaken the model performance as compared to the TA model. From this aspect,
325 the greater deviation from a linear relationship between the $M_{\hat{tn}}$ and EOF1 of the
326 R_{tn} , may lead to a greater outperformance of the TA model over the SA model.
327 Finally, the performances of both models rely on the estimation accuracy of the EC_t ,
328 which depends on both goodness of fit of the cosine function (i.e., Eq. 4) and

329 estimation accuracy of the S_{in} . Because the same S_{in} values are used for the two
330 models, the relative performance of the two models is related to the goodness of fit of
331 Eq. (4).

332 **3. Results**

333 **3.1 Components of SWC and their controls**

334 **3.1.1 Spatial mean (S_{in}) and spatial anomaly (Z_{in})**

335 The values of spatial mean (S_{in}) in the SA model varied with the seasons (Fig. 3a).
336 In the spring, such as May 2, 2008 and April 20, 2009, snowmelt infiltration resulted
337 in relatively great S_{in} values. In the summer, however, even one month after large
338 rainfall events (such as on July 19, 2008 and June 21, 2009), the high
339 evapotranspiration by fast-growing vegetation resulted in small S_{in} values. The
340 values of S_{in} also varied between inter-annual meteorological conditions. In 2008,
341 there was less precipitation and higher air temperature than in 2010 (Fig. 2). As a
342 result, S_{in} was relatively smaller in 2008 than in 2010.

343 The spatial patterns of spatial anomaly (Z_{in}) were similar to those of the original
344 SWC patterns (Fig. 3a). The values of Z_{in} in wet periods (e.g., May 13, 2011) were
345 much greater than in dry periods (e.g., August 23, 2008) in depressions (e.g., at a
346 distance of 123 and 250 m); at other locations, however, the spatial anomaly was
347 slightly less in wet periods than in dry periods for both soil layers. Moreover, the
348 spatial anomaly in depressions during the wet periods was much greater in the near
349 surface than in the root zone.

350 When SWCs of all 23 dates were used for model development, only EOF1 was
 351 statistically significant (Fig. 4a), which accounted for 84.3% (0–0.2 m) and 86.5%
 352 (0–1.0 m) of the variances in the Z_{in} . Correlation analysis indicated that the spatial
 353 pattern of EOF1 in the Z_{in} was identical to the time-stable patterns ($M_{\hat{in}}$) in the TA
 354 model ($R=1.0$). The controls of EOF1 was therefore the same as those of $M_{\hat{in}}$, and
 355 will be discussed later. The relationship between associated EC1 and $S_{\hat{in}}$ can be
 356 fitted well by the cosine function ($R^2=0.73$ at both the near surface and root zone) (Fig.
 357 4b).

358 **3.1.2 Time-stable pattern ($M_{\hat{in}}$), space-invariant temporal anomaly ($A_{\hat{in}}$), and**
 359 **space-variant temporal anomaly (R_{in})**

360 Figure 3b displays the three components in the TA model. The first component
 361 $M_{\hat{in}}$ fluctuated along the transect, with high values in depressions and low values on
 362 knolls; the $M_{\hat{in}}$ also had greater spatial variability in the near surface (variance
 363 $=36.7\%^2$) than in the root zone (variance $=19.5\%^2$). For both soil layers, SOC, depth to
 364 the CaCO_3 layer, sand content, and wetness index are the dominant factors of $M_{\hat{in}}$;
 365 they together explained 74.5% (near surface) and 75.6% (root zone) of the variances
 366 in the $M_{\hat{in}}$ (Table 1). In addition, the temporal trend of $A_{\hat{in}}$ was the same as that of
 367 $S_{\hat{in}}$ in the SA model (Fig. 3a) as both represent temporal forcing.

368 The R_{in} varied among landscape positions (Fig. 3b). At a sampling distance of
 369 123 m (in a depression), R_{in} was negative in dry periods such as August 23, 2008 and
 370 positive in wet periods such as May 13, 2011. This was true for all depressions for
 371 both the near surface and the root zone. Therefore, topographically lower positions

372 usually corresponded to more positive R_m during the wet periods and more negative
373 R_m during the dry periods. Furthermore, the absolute values of R_m were generally
374 greater in the near surface than the root zone, indicating a greater space-variant
375 temporal anomaly for shallower depths.

376 The SWC variances and associated components (Eq. 8) also varied with time (Fig.
377 5). Often, wetter conditions corresponded to greater $\sigma_n^2(S_m)$, as further indicated by
378 moderate correlation between $\sigma_n^2(S_m)$ and S_m (R^2 of 0.51 and 0.38 for the near
379 surface and the root zone, respectively). This was in agreement with others
380 (Gómez-Plaza et al., 2001; Martínez-Fernández and Ceballos, 2003; Hu et al., 2011).
381 Furthermore, there were greater $\sigma_n^2(S_m)$ values at near surface than in the root zone,
382 indicating greater variability of SWC in the near surface.

383 The time-invariant $\sigma_n^2(M_m)$ accounted for the $\sigma_n^2(S_m)$ with percentages
384 ranging from 25 to 795% for the near surface and from 40 to 174% for the root zone
385 (Fig. 5). The $\sigma_n^2(M_m)$ exceeded the $\sigma_n^2(S_m)$ mainly under dry conditions, such as
386 July–October in 2008 and 2009. This excess was offset by the $\sigma_n^2(R_m)$ and
387 $2\text{cov}(M_m, R_m)$, with the latter accounting for the $\sigma_n^2(S_m)$ negatively with mean
388 absolute percentages of 210% for the near surface and 17% for the root zone. In the
389 dry period, the absolute percentage of $2\text{cov}(M_m, R_m)$ was up to 1327% for the near
390 surface and 122% for the root zone. These values are comparable to those in
391 Mittelbach and Seneviratne (2012) and Brocca et al. (2014).

392 The $\sigma_n^2(R_m)$ accounted for less percentage of the $\sigma_n^2(S_m)$ than other

393 components did (Fig. 5). The percentages of $\sigma_{\hat{n}}^2(R_m)$ ranged from 11 to 632%
394 (arithmetic average of 118%) for the near surface and from 6 to 48% (arithmetic
395 average of 19%) for the root zone; the percentage of $\sigma_{\hat{n}}^2(R_m)$ tended to be greater in
396 drier periods. This indicates that the space-variant temporal anomaly cannot be
397 ignored, particularly in dry conditions. Furthermore, the percentage of $\sigma_{\hat{n}}^2(R_m)$ was
398 greater in the near surface than in the root zone, confirming stronger temporal
399 dynamics of soil water at the near surface. Compared with larger scale studies
400 (Mittelbach and Seneviratne, 2012; Brocca et al., 2014), the percentage of $\sigma_{\hat{n}}^2(R_m)$
401 out of the $\sigma_{\hat{n}}^2(S_m)$ at the near surface was greater, with a mean percentage of 118%,
402 versus 9–68% in the other, larger scale studies. This indicates that interactions
403 between spatial and temporal forcing were stronger, resulting in relatively more
404 intensive temporal dynamics of soil water in our study area than at larger scales.

405 Three significant EOFs of R_m for both soil layers were identified when SWC of
406 all 23 dates were used for model development. The first three EOFs explained 61.1,
407 13.4, and 8.1% respectively, of the total R_m variance for the near surface, and 44.3,
408 20.2, and 12.4%, respectively, of the total R_m variance in the root zone. Therefore,
409 our hypothesis that underlying spatial patterns exist in the R_m was supported. Due
410 to the negligible contribution of EOF2 and EOF3 to the estimation of spatially
411 distributed SWC, only EOF1 is shown in Fig. 6a. The associated EC1 changed with
412 soil water conditions (S_m) (Fig. 6b). When SWC was close to average levels, the EC1
413 was close to 0, resulting in negligible R_m . This was in accordance with Mittelbach
414 and Seneviratne (2012) and Brocca et al. (2014), who showed that the spatial variance

415 of the temporal anomaly was the smallest when water contents were close to average
416 levels. The cosine function (Eq. 4) explained a large amount of the variances in EC1
417 for both soil layers ($R^2=0.76$ at the near surface and 0.88 in the root zone).

418 The contribution of EOF1 to the space-variant temporal anomaly can be examined
419 through the product of the EOF1 and the associated EC1. The EC1 values tended to
420 be positive during wet periods and negative during dry periods (Fig. 6b); more
421 positive EOF1 values were usually observed at locations with greater $M_{\hat{m}}$ values
422 (Figs. 3b and 6a). Therefore, the product of EOF1 and EC1 led to greater temporal
423 SWC dynamics at wetter locations of both layers in both the wet and dry periods.

424 Depth to the CaCO_3 layer and SOC had significant, positive correlations with
425 EOF1 for both soil layers (R ranging from 0.76 to 0.88; Table 1). They jointly
426 accounted for 81.6% (near surface) and 81.0% (root zone) of the variances in EOF1.
427 This implies that locations with a greater depth to the CaCO_3 layer and SOC, which
428 correspond to wetter locations such as depressions, usually have greater temporal
429 SWC dynamics during both wet and dry periods.

430 **3.2 Estimation of spatially distributed SWC**

431 When all 23 datasets were used and only EOF1 was considered, the TA model had
432 an AICc value of 4093 for the near surface and 562 for the root zone, while the
433 corresponding values for the SA model were 6370 and 3460. This indicated that even
434 when penalty to complexity was given, the TA model was better than the SA model.
435 The two models in terms of spatially distributed SWC estimation are compared below.

436 **3.2.1 The TA model**

437 The R_m terms and associated EOFs differed slightly with each validation. The
438 number of significant EOFs varied between one (accounting for 60% of the total cases)
439 and three for both soil layers. A paired samples T-test indicated that more EOFs did
440 not result in a significant increase of NSCE in the estimation of spatially distributed
441 SWC for both validation methods. This is also supported by the increasing AICc
442 values with the increasing number of parameters resulting from more EOFs (data not
443 shown). This indicates that higher-order EOFs, even if they are statistically significant,
444 are negligible for SWC prediction. Therefore, SWC distribution was estimated with
445 EOF1 only.

446 Estimated SWCs generally approximated those measured at different soil water
447 conditions during the cross validation (Fig. 7). However, on October 27, 2009, there
448 were unsatisfactory overestimates at the 100–140 and 220–225 m locations near the
449 surface (Fig. 7a). Unsatisfactory NSCE values of -4.05, -1.83, and -3.81 were
450 obtained in the near surface in only three of the 23 dates, which were all in the fall
451 (October 22, 2008, August 27, 2009, and October 27, 2009, respectively). The poor
452 performance obtained with the TA model on those dates (Fig. 8a) was a result of
453 overestimation in depressions, which is shown for example on October 27, 2009 (Fig.
454 7a). These dates also corresponded to a high percentage of $\sigma_{\hat{n}}^2(R_m)$ to the $\sigma_{\hat{n}}^2(S_m)$
455 (203–439%). For August 23 and September 17 in 2008, which were in dry periods,
456 the percentage of $\sigma_{\hat{n}}^2(R_m)$ at the near surface was also high (580 and 630%).
457 Because a fair amount of $\sigma_{\hat{n}}^2(R_m)$ was accounted for with the TA model, the TA
458 model performed satisfactorily (NSCE of 0.43 and 0.60). For the remaining 20 dates,

459 the resulting NSCE value ranged from 0.38 to 0.90 in the near surface and from 0.65
460 to 0.96 in the root zone (Fig. 8). This suggests that the TA model was generally
461 satisfactory, with better performance in the root zone than in the near surface.

462 During the split sample validation, the TA model resulted in SWC estimations with
463 NSCE values ranging from 0.61 to 0.85 near the surface and from 0.32 to 0.92 in the
464 root zone, with exception of two days (August 27, 2009 and October 27, 2009 with
465 NSCE values of -2.63 and -5.12, respectively) at 0–0.2 m (Fig. 8). This suggested that
466 the TA model performed well in estimating spatially distributed SWC patterns except
467 on August 27, 2009 and October 27, 2009 at 0–0.2 m. The estimation in the root zone
468 was also generally better than in the near surface.

469 **3.2.2 Comparison with the SA model**

470 One significant EOF of Z_{in} was identified for both soil layers, irrespective of the
471 validation method. The SA model with only EOF1 produced reasonable SWC
472 estimations for both validations in all dates in the root zone and in every date except
473 five dates (August 23, 2008, September 17, 2008, October 22, 2008, August 27, 2009,
474 and October 27, 2009) in the near surface (Fig. 8). Similarly, when more EOFs were
475 included, NSCE values did not increase significantly (data not shown) and
476 consequently, estimation of spatially distributed SWC was not improved. This was
477 because EOF2 and EOF3 together explained a very limited (<10%) amount of
478 variability of Z_{in} and thus had low predictive power in terms of variance.

479 The difference in NSCE values between the TA and SA models for both validations
480 are presented in Fig. 9. Generally, the difference decreased as A_{in} increased, and

481 then slightly increased with a further increase in $A_{\hat{m}}$. A paired samples T-test
482 indicated that the NSCE values of the TA model were significantly ($P<0.05$) greater
483 than those of the SA model for both soil layers, irrespective of validation methods.
484 This indicates that the TA model outperformed the SA model, particularly in dry
485 conditions. This was because when the soil was dry, there was a high percentage of
486 $\sigma_{\hat{n}}^2(R_m)$, and thus strong variability in the space-variant temporal anomaly.

487 **3.3 Further application at other two sites with different scales**

488 **3.3.1 A hillslope in the Chinese Loess Plateau**

489 On average, the $\sigma_{\hat{n}}^2(M_{\hat{m}})$, $\sigma_{\hat{n}}^2(R_m)$, and $2\text{cov}(M_{\hat{m}}, R_m)$ accounted for 53, 74
490 and -27% out of the $\sigma_{\hat{n}}^2(S_m)$, indicating that both time-stable pattern and temporal
491 anomalies were the main contributors to the $\sigma_{\hat{n}}^2(S_m)$. The EOF analysis showed that
492 only the EOF1 was statistically significant for both the R_{tm} and Z_{tm} , and the EOF1
493 explained 23% and 47% of the total variances of R_{tm} and Z_{tm} , respectively. This
494 illustrated that underlying spatial patterns exist in the R_{tm} on the hillslope. Cross
495 validation was used to estimate the spatially distributed SWC along the hillslope. The
496 results showed that the NSCE varied from -4.25 to 0.83 (TA model) and from -4.30 to
497 0.81 (SA model), with a mean value of 0.25 and 0.19, respectively (Fig. 10a). A paired
498 samples T-test showed that the NSCE values for the TA model were significantly
499 ($P<0.05$) greater than those for the SA model, indicating that the TA model
500 outperformed the SA model. As Fig. 10a shows, the outperformance was greater when
501 SWC deviated from intermediate conditions, especially for dry conditions, which was
502 similar to the Canadian site.

503 3.3.2 The GENCAI network in Italy

504 The $\sigma_{\hat{n}}^2(M_{\hat{m}})$, $\sigma_{\hat{n}}^2(R_m)$, and $2\text{cov}(M_{\hat{m}}, R_m)$ accounted for 38, 68, and -7% out
505 of the $\sigma_{\hat{n}}^2(S_m)$ (Brocca et al., 2014), indicating the dominant role of temporal
506 anomalies in SWC variability. The first three EOFs of the R_m explained 19, 16, and
507 8% of the total $\sigma_{\hat{n}}^2(R_m)$, and no EOFs were statistically significant, indicating that no
508 underlying spatial patterns exist in the R_m . The EOF1 of the Z_m was significant
509 and accounted for 37% of the variances in the Z_m . Although the EOF1 of the R_m
510 was not significant, it was considered in the TA model for estimating spatially
511 distributed SWC. The cross validation indicates that the NSCE varied from -0.79 to
512 0.50 (TA model) and from -0.87 to 0.56 (SA model), with mean values of 0.09 and
513 0.08, respectively (Fig. 10b). The SWC estimation based on these two models was not
514 satisfactory except for a few days. As Fig. 10b shows, the differences in NSCE values
515 between the two models were scattered around 0. A paired samples T-test showed that
516 the NSCE values between the TA model and the SA model were not significant
517 ($P < 0.05$), indicating no differences in estimating spatially distributed SWC between
518 these two models.

519 4 Discussion

520 4.1 Controls of the $M_{\hat{m}}$ and R_m

521 The R_m played an important role in the temporal change in spatial patterns of the
522 SWC. The underlying spatial patterns and physical meaning in the R_m were
523 examined in our study for the first time. Although three significant EOFs of the R_m

524 existed in some cases, only EOF1 rather than higher-order EOFs of the R_m should
525 be considered for the spatially distributed SWC estimation. Among many factors
526 influencing the EOF1 of the R_m , depth to the CaCO_3 layer followed by the SOC,
527 were the most important factors. Depressions have deeper CaCO_3 layers than knolls,
528 and the shallow CaCO_3 layer on knolls limited water infiltration during rainfall or
529 snowmelt, resulting in less water recharge on knolls than in depressions. The depth to
530 CaCO_3 layer and SOC were negatively correlated with elevation ($R=-0.54$, $P<0.01$).
531 Therefore, the influence of depth to CaCO_3 layer and SOC partially reflected the role
532 of topography in driving snowmelt runoff along slopes in the spring, which
533 contributes to increasing water recharge in depressions. As already demonstrated,
534 topographically lower positions corresponded to more negative R_m during the dry
535 periods. This implies that depressions lost more water during discharge. This is
536 because depressions usually corresponded to vegetation with a larger leaf area index,
537 which would result in higher evapotranspiration and more water loss during discharge
538 periods.

539 As Table 1 shows, both the depth to the CaCO_3 layer and SOC controlled the $M_{\hat{m}}$.
540 This was because deeper CaCO_3 layers and higher SOC were observed in depressions
541 where soils were usually wetter in most of the year because of the snowmelt runoff in
542 the spring and rainfall runoff in the summer and autumn (van der Kamp et al., 2003).
543 Therefore, the roles of soil and topography were two-fold: On one hand, they were
544 highly correlated with the time-stable patterns and thus the time stability of SWC
545 (Gómez-Plaza et al., 2000; Mohanty and Skaggs, 2001; Grant et al., 2004); On the

546 other hand, soil and topography, interplaying with temporal forcing, triggered
547 local-specific soil water change and destroyed time stability of SWC. Their roles in
548 protecting time stability persisted, but their roles in destroying time stability varied
549 with time. Greater $\sigma_{\hat{n}}^2(R_m)$ implies greater contribution of these factors in soil water
550 dynamics, resulting in less time stability of SWC.

551 **4.2 Model performance for spatially distributed SWC estimation**

552 The outperformance of the TA model for estimating spatial SWC at the Canadian
553 site and Chinese site can be partly explained by the high percentages (average of
554 19–118%) of the $\sigma_{\hat{n}}^2(R_m)$ out of the total variance. When SWC is close to average
555 levels, R_m is also close to zero, resulting in negligible percentage of $\sigma_{\hat{n}}^2(R_m)$. In
556 this case, the soil water patterns are stable in time, the SA model performs well, and
557 there will be little differences between these two models. As is well known, the spatial
558 patterns in soil water content are inherently time unstable. For example, when
559 evapotranspiration becomes the dominant process at the small watershed scale, more
560 water will be lost in depressions due to the denser vegetation than on knolls (Millar,
561 1971; Biswas et al., 2012), effectively diminishing the spatial patterns and increasing
562 temporal instability. In this case, the $\sigma_{\hat{n}}^2(R_m)$ accounts for more percentage of the
563 total variance (e.g., high up to 632%) and the TA model may outperform the SA
564 model. This explained why the outperformance of the TA model was more obvious in
565 the dry conditions. For the GENCAI network in Italy, although the $\sigma_{\hat{n}}^2(R_m)$
566 accounted for 68% of the total variance, the performance of the TA model was
567 identical to the SA model. This was because there were no underlying spatial patterns

568 in the R_{tm} . Similarly, because the first underlying spatial pattern (i.e., EOF1)
569 explained greater percentages of the $\sigma_{\hat{n}}^2(R_m)$ at the Canadian site (44–61%) than the
570 Chinese site (23%), the outperformance of the TA model over the SA model was more
571 obvious at the former site (Fig. 9 and 10a). Therefore, the TA model is advantageous
572 only if the percentage of $\sigma_{\hat{n}}^2(R_m)$ out of the total variance is substantial and
573 underlying spatial patterns exist in the R_{tm} .

574 The existence of underlying spatial patterns in the R_{tm} is related to the controlling
575 factors, which may be scale-specific. At small scales, “static” factors such as the depth
576 to the CaCO_3 layer and SOC at the Canadian site may affect not only the time-stable
577 patterns but also the R_{tm} . The persistent influence of “static” factors on the R_{tm}
578 resulted in significant underlying spatial patterns in the R_{tm} . Thus, the TA model
579 outperformed the SA model at the small scales. At large scales such as the basin scale
580 or greater, time-stable patterns may be controlled by, in addition to soil and
581 topography (Mittelbach and Seneviratne, 2012), the climate gradient (Sherratt and
582 Wheeler, 1984); at those scales, R_{tm} is more likely to be controlled by the
583 meteorological anomaly (i.e., spatially random variation) (Walsh and Mostek, 1980),
584 and the effects of soil and topography may be reduced. Consequently, spatial patterns
585 in the R_{tm} may be weakened and the TA model may have no advantages over the SA
586 model such as for the Italian site.

587 The $M_{\hat{m}}$ and the underlying spatial patterns (EOF1) in the R_{tm} were controlled
588 by the same spatial forcing (e.g., depth to CaCO_3 layer and SOC) at the Canadian site
589 (Table 1), and they were correlated with an R^2 of 0.83 for the near surface and 0.42 for

590 the root zone. Although the relationships between $M_{\hat{m}}$ and R_m were strong, they
591 were not strictly linear, suggesting that $M_{\hat{m}}$ and R_m were affected differently by
592 these factors. Therefore, the nonlinear relationship between $M_{\hat{m}}$ and R_m partially
593 contributed to the outperformance of the TA model over the SA model.

594 The relationship between the $S_{\hat{m}}$ and EC1 was better fitted by the cosine function
595 in the TA model than the SA model (Figs. 4b and 6b), with R^2 of 0.76 versus 0.73 in
596 the near surface and 0.88 versus 0.73 in the root zone. The reduced scatter in the $S_{\hat{m}}$
597 and EC1 relationship for the TA model may also partly explain the outperformance of
598 the TA model over the SA model.

599 Therefore, the outperformance of the TA model over the SA model depends on
600 counterbalance among the variance of R_m explained in the TA model, the linear
601 correlation between the $M_{\hat{m}}$ and EOF1 of the R_m , and the goodness of fit for the
602 $S_{\hat{m}}$ and EC1 relationship. For example, the variance of EOF1 in the R_m for the
603 near surface (i.e., 264%²) was much greater than that for the root zone (i.e., 43%²).
604 However, $M_{\hat{m}}$ and underlying spatial patterns (EOF1) in the R_m in the root zone
605 deviated more from a linear relationship, and the reduced scatter in the $S_{\hat{m}}$ and EC1
606 relationship in the TA model was more obviously in the root zone than in the near
607 surface. As a result, the outperformance of the TA model was comparable between the
608 near surface and root zone at the Canadian site (Fig. 9).

609 In the real world, the relations between the $M_{\hat{m}}$ and underlying spatial patterns in
610 the R_m may rarely be perfectly linear. Therefore, when underlying spatial patterns
611 exist in the R_m and the R_m has substantial variances, the TA model is preferable

612 to the SA model for the estimation of spatially distributed SWC. On the contrary,
613 when underlying spatial patterns does not exist in the R_m or the R_m has negligible
614 variances, the SA model may be selected although these two models yield the same
615 quality of SWC estimation. This is because the TA model needs one more spatial
616 parameter (i.e., $M_{\hat{m}}$) than the SA model.

617 Previous studies on SWC decomposition mainly focus on near surface layers
618 (Jawson and Niemann, 2007; Perry and Niemann, 2007, 2008; Joshi and Mohanty,
619 2010; Korres et al., 2010; Busch et al., 2012). This study decomposed spatiotemporal
620 SWC using the TA model for both the near surface and the root zone. The results
621 showed that the estimation of spatially distributed SWC at small watershed scales was
622 improved by the TA method that considers the R_m . The $\sigma_n^2(M_{\hat{m}})$ was greater than
623 the $\sigma_n^2(R_m)$ (Fig. 5), indicating that time stability was more important than time
624 instability for SWC estimation. For the three dates in the fall (i.e., October 22, 2008,
625 August 27, 2009, and October 27, 2009), strong evapotranspiration and deep drainage
626 in depressions resulted in a much lower SWC at the near surface than in the spring.
627 This resulted in reduced time stability of SWC pattern and poor performance of both
628 models and validation methods in terms of SWC evaluation (Fig. 8a). Because of the
629 stronger time stability of SWC in deeper soil layers (Biswas and Si, 2011), SWC
630 evaluation was more accurate for soil layers extending from the surface to greater
631 depth. This is particularly important because SWC data for deeper soil layers in a
632 watershed is more difficult to collect than that of surface soil.

633 5 Conclusions

634 The TA model was used to decompose spatiotemporal SWC into time-stable
635 patterns $M_{\hat{m}}$, space-invariant temporal anomaly $A_{\hat{m}}$, and space-variant temporal
636 anomaly R_m . This study indicated that underlying spatial patterns may exist in the
637 R_m at small scales (e.g., small watersheds and hillslope) but may not exist at large
638 scales such as the GENCAI network (~250 km²) in Italy. This was because the R_m
639 at small scales was driven by “static” factors such as depth to the CaCO₃ layer and
640 SOC at the Canadian site, while the R_m at large scales may be dominated by
641 “dynamic” factors such as meteorological anomaly. Compared to the SA model,
642 estimation of spatially distributed SWC was improved with the TA model at small
643 watershed scales. This was because the TA model considered a fair amount of spatial
644 variance in the R_m , which was ignored in the SA model. Furthermore, the improved
645 performance was observed mainly when there was less or more soil water than the
646 average level, especially in drier conditions due to the high $\sigma_{\hat{n}}^2(R_m)$ value.

647 This study showed that outperformance of the TA model over the SA model is
648 possible when $\sigma_{\hat{n}}^2(R_m)$ accounts for substantial variance of SWC, and significant
649 spatial patterns (or EOFs) exist in the R_m . Further application of the TA model for
650 the estimation of spatially distributed SWC at different scales and hydrological
651 backgrounds is recommended. If the TA model parameters (i.e., $M_{\hat{m}}$, EOF1 of the
652 R_m , and relationship between EC and $S_{\hat{m}}$) are obtained from historical in-situ SWC
653 datasets, a detailed spatially distributed SWC of near surface soil at watershed scales
654 can be constructed from remotely sensed SWC. Note that both models rely on

655 in-situ SWC measurements for model parameters. Therefore, future research should
656 be conducted to estimate spatially distributed SWC in un-gauged watersheds based on
657 the estimation of the model parameters using pedotransfer functions. The codes for
658 decomposing SWC with the SA and TA models and related EOF analysis were written
659 in Matlab and are freely available from the authors upon request.

660 **Acknowledgements**

661 This project was funded by the National Science Foundation of China (K305021308)
662 and the Natural Sciences and Engineering Research Council (NSERC) of Canada. We
663 thank Dr. Asim Biswas, Dr. Henry Wai Chau, Mr. Trent Pernitsky, and Mr. Eric Neil
664 for their help in data collection. We thank the anonymous reviewers and the Editor for
665 their constructive comments.

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808 **Figure captions**

809 **Figure 1.** Decomposition of spatiotemporal soil water content (SWC) in different
810 models.

811 **Figure 2.** Daily mean air temperature and precipitation during the study period.

812 **Figure 3.** Components of soil water content in (a) the SA model (spatial mean soil
813 water content $S_{\hat{m}}$ and spatial anomaly Z_{tm}) and in (b) the TA model (time-stable
814 pattern $M_{\hat{m}}$, space-invariant temporal anomaly $A_{\hat{m}}$, and space-variant temporal
815 anomaly R_{tm}) for 0–0.2 and 0–1.0 m. Also shown is the elevation.

816 **Figure 4.** (a) The EOF1 of the spatial anomaly Z_{tm} and (b) relationships of
817 associated EC1 versus spatial mean soil water content Z_{tm} fitted by the cosine
818 function (Eq. 4).

819 **Figure 5.** Spatial variances of different components in Eq. (8) expressed in %² (upper
820 panel) and as percentage (lower panel) for (a) 0–0.2 and (b) 0–1.0 m. Spatial mean
821 soil water content $S_{\hat{m}}$ on each measurement day is also shown.

822 **Figure 6.** (a) The EOF1 of the space-variant temporal anomaly R_{tm} and (b)
823 relationships of associated EC1 versus spatial mean soil water content $S_{\hat{m}}$ fitted by
824 the cosine function (Eq. 4).

825 **Figure 7.** Estimated soil water content (SWC) versus measured SWC for three dates
826 at different soil water conditions (August 23, 2008, October 27, 2009, and May 13,
827 2011 are associated with relatively dry, medium, and wet days, respectively) using the
828 TA model for (a) 0–0.2 and (b) 0–1.0 m.

829 **Figure 8.** The Nash-Sutcliffe coefficient of efficiency (NSCE) of soil water content

830 estimation using the TA and SA models for (a) 0–0.2 and (b) 0–1.0 m for both cross
831 validation (CV) and split sample validation (SV). At 0–0.2 m, three dates (October 22,
832 2008, August 27, 2009, and October 27, 2009) as indicated by green lines present
833 negative NSCE values (-4.05, -1.83, and -3.81, respectively, for the CV on the three
834 dates; -2.63 and -5.12, respectively, for the SV on the latter two dates). Spatial mean
835 soil water content $S_{\hat{m}}$ on each measurement day is also shown.

836 **Figure 9.** Nash-Sutcliffe coefficient of efficiency (NSCE) difference between the TA
837 and SA models in terms of soil water content estimation using both cross validation
838 (CV) and split sample validation (SV) as a function of space-invariant temporal
839 anomaly $A_{\hat{m}}$ for (a) 0–0.2 and (b) 0–1.0 m.

840 **Figure 10.** Nash-Sutcliffe coefficient of efficiency (NSCE) difference between the TA
841 and SA models in terms of soil water content estimation using cross validation as a
842 function of space-invariant temporal anomaly $A_{\hat{m}}$ for (a) 0–0.06 m of the Chinese
843 Loess Plateau hillslope and (b) 0–0.15 m of the GENCAI network in Italy. The NSCE
844 values for both models are also shown.

Table 1. Pearson correlation coefficients between time-stable pattern $M_{\hat{t}n}$, EOF1 of space-variant temporal anomaly R_{tn} and various properties.

| | 0–0.2 m | | 0–1.0 m | |
|----------------------------------|----------------|---------|----------------|---------|
| | $M_{\hat{t}n}$ | EOF1 | $M_{\hat{t}n}$ | EOF1 |
| Sand content | -0.52** | -0.36** | -0.66** | -0.26** |
| Silt content | 0.29** | 0.14 | 0.40** | 0.06 |
| Clay content | 0.43** | 0.38** | 0.51** | 0.33** |
| Organic carbon | 0.78** | 0.83** | 0.73** | 0.76** |
| Wetness index | 0.64** | 0.59** | 0.68** | 0.56** |
| Depth to CaCO ₃ layer | 0.77** | 0.84** | 0.65** | 0.88** |
| A horizon depth | 0.51** | 0.62** | 0.44** | 0.65** |
| C horizon depth | 0.66** | 0.69** | 0.58** | 0.76** |
| Bulk density | -0.58** | -0.67** | -0.46** | -0.62** |
| Elevation | -0.24** | -0.28** | -0.24** | -0.32** |
| Specific contributing area | 0.20* | 0.24** | 0.24** | 0.23** |
| Convergence index | -0.58** | -0.56** | -0.55** | -0.58** |
| Curvature | -0.10 | -0.08 | -0.19* | -0.16 |
| Cos(aspect) | 0.05 | 0.04 | 0.08 | 0.05 |
| Gradient | -0.12 | -0.09 | -0.21* | -0.02 |
| Slope | -0.51** | -0.48** | -0.56** | -0.44** |
| Upslope length | 0.19* | 0.21* | 0.21* | 0.25** |
| Solar radiation | -0.07 | 0.03 | -0.11 | 0.08 |
| Flow connectivity | 0.45** | 0.43** | 0.49** | 0.49** |
| Leaf area index | -0.07 | 0.06 | -0.10 | -0.14 |
| Variance explained ¹ | 74.5% | 81.6% | 75.6% | 81.0% |

¹percent of variance explained by the controlling factors obtained by the multiple stepwise regressions.

*Significant at $P<0.05$; ** Significant at $P<0.01$.

Table A1. Notations.

| | |
|----------------------|--|
| $M_{\hat{m}}$ | spatial mean of $M_{\hat{m}}$ |
| R_{tn} | space-variant temporal anomaly of SWC at location n and time t |
| $A_{\hat{m}}$ | space-invariant temporal anomaly of SWC at time t |
| Z_{tn} | spatial anomaly of SWC at location n and time t |
| $S_{\hat{m}}$ | spatial mean SWC at time t |
| $\sigma_{\hat{n}}^2$ | spatial variance |
| A_{tn} | temporal anomaly of SWC at location n and time t |
| $\delta_{\hat{m}}$ | temporal mean relative difference of SWC at location n |
| COV | spatial covariance |
| S_{tn} | SWC at location n and time t |
| $M_{\hat{m}}$ | time-stable pattern of SWC |
| ECs | temporally-varying coefficients of R_{tn} (or Z_{tn}) |
| EOFs | time-invariant spatial structures of R_{tn} (or Z_{tn}) |
| NSCE | Nash-Sutcliffe coefficient of efficiency |
| R | Pearson correlation coefficient |
| SWC | soil water content |

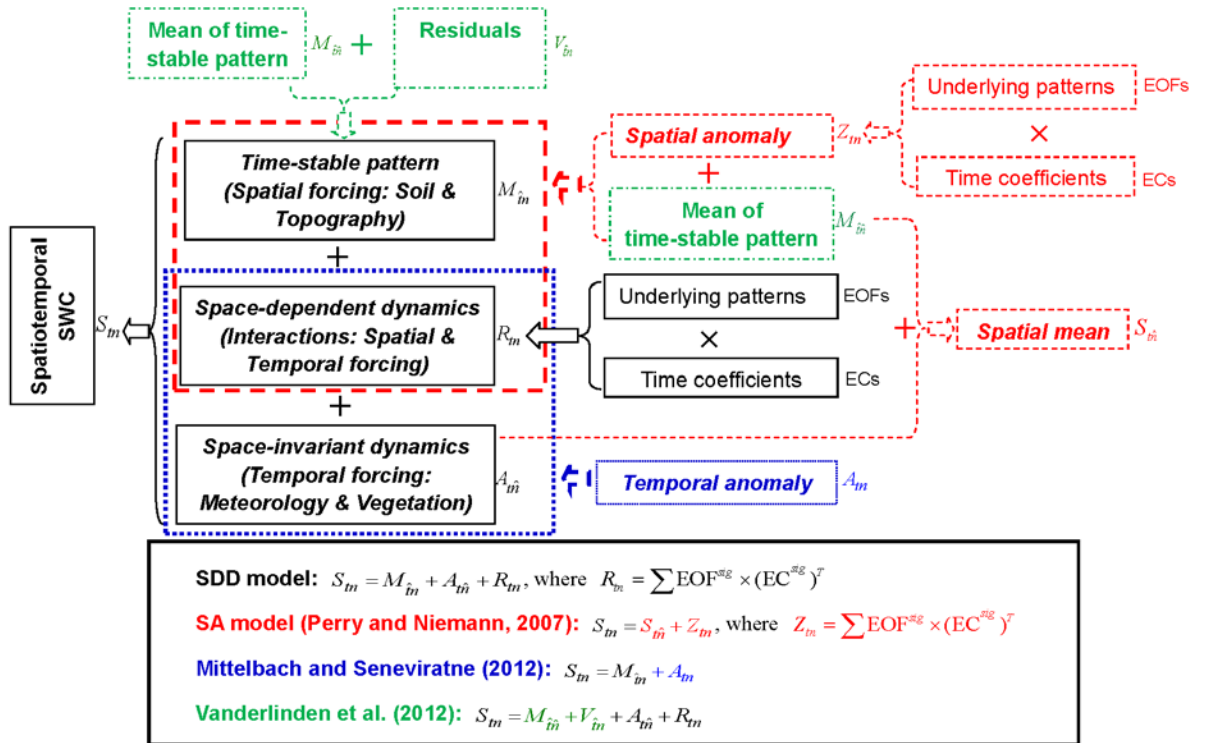


Fig. 1. Decomposition of spatiotemporal soil water content (SWC) in different models.

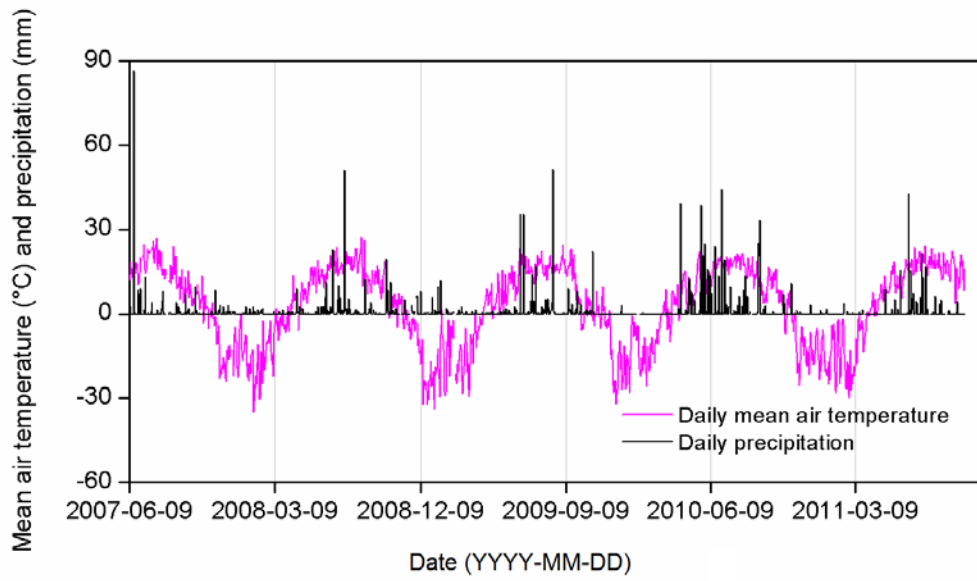


Fig. 2. Daily mean air temperature and precipitation during the study period.

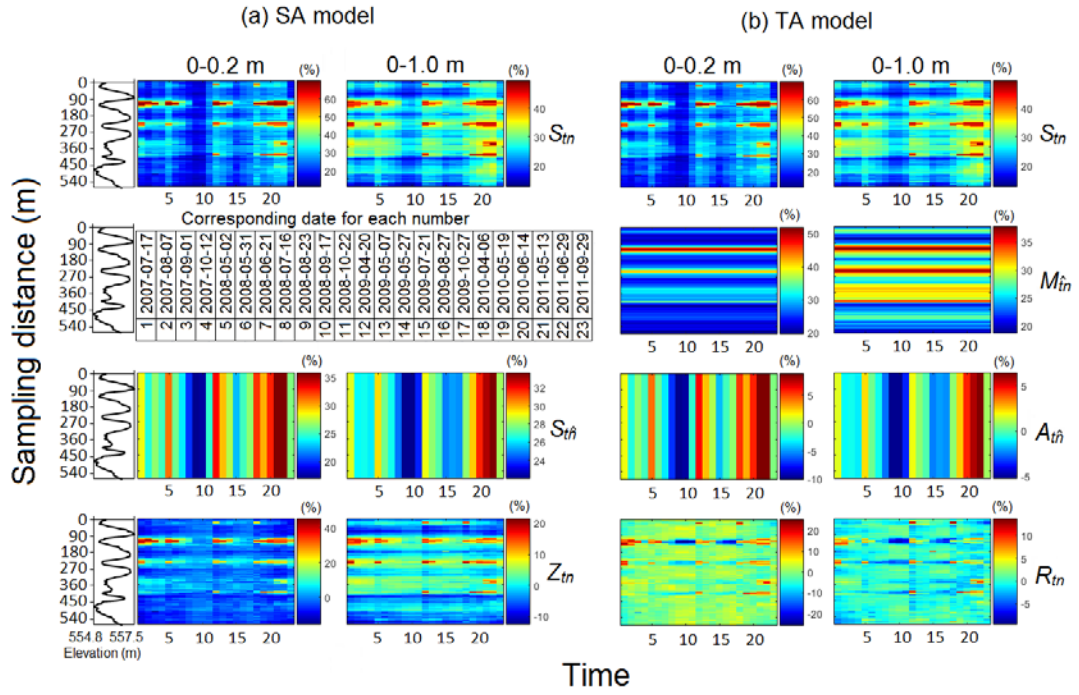


Fig. 3. Components of soil water content in (a) the SA model (spatial mean soil water content $S_{\hat{m}n}$ and spatial anomaly $Z_{\hat{m}n}$) and in (b) the TA model (time-stable pattern $M_{\hat{m}n}$, space-invariant temporal anomaly $A_{\hat{m}n}$, and space-variant temporal anomaly $R_{\hat{m}n}$) for 0–0.2 and 0–1.0 m. Also shown is the elevation.

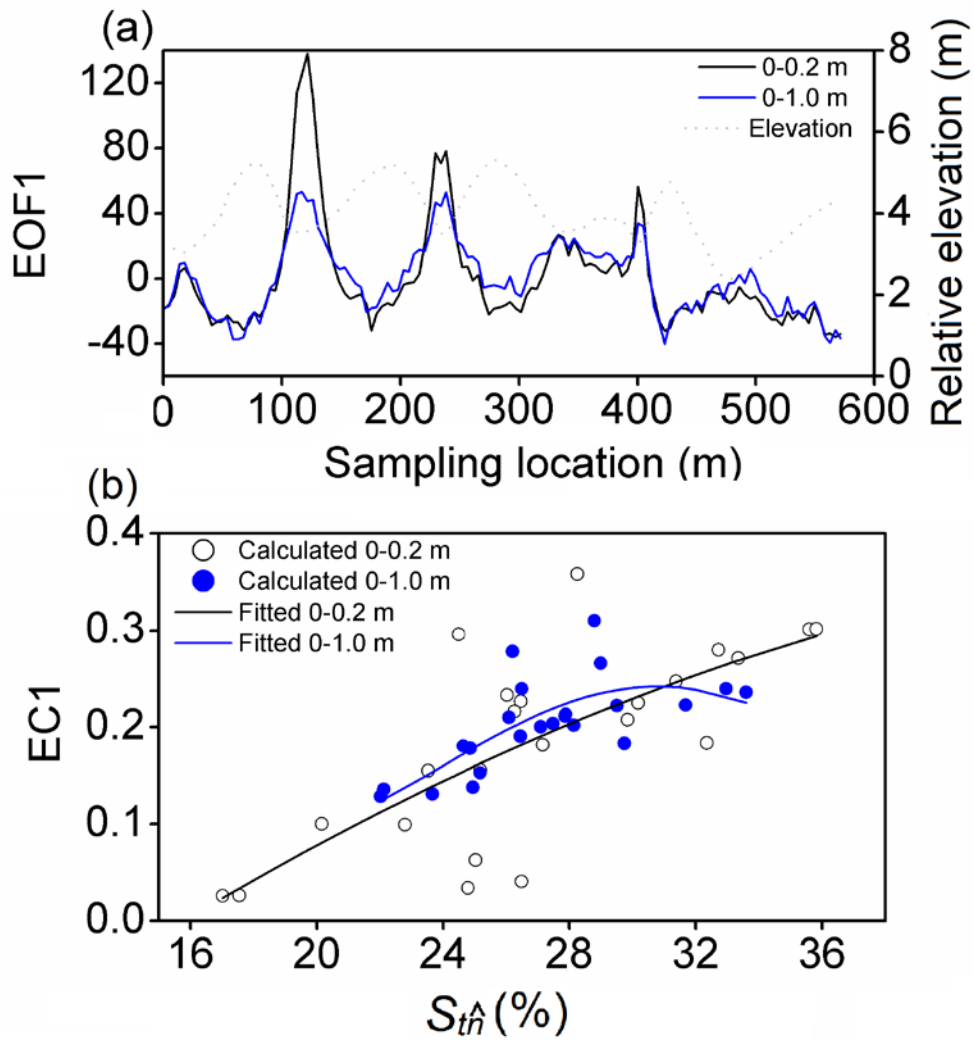


Fig. 4. (a) The EOF1 of the spatial anomaly Z_m and (b) relationships of associated EC1 versus spatial mean soil water content Z_m fitted by the cosine function (Eq. 4).

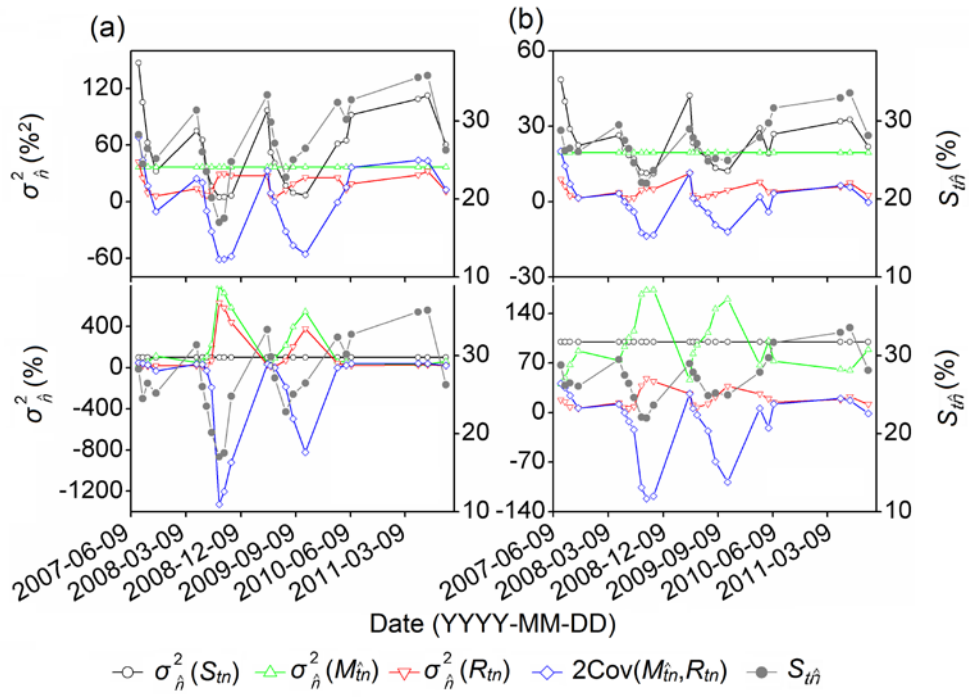


Fig. 5. Spatial variances of different components in Eq. (8) expressed in $\%^2$ (upper panel) and as percentage (lower panel) for (a) 0–0.2 and (b) 0–1.0 m. Spatial mean soil water content S_{it} on each measurement day is also shown.

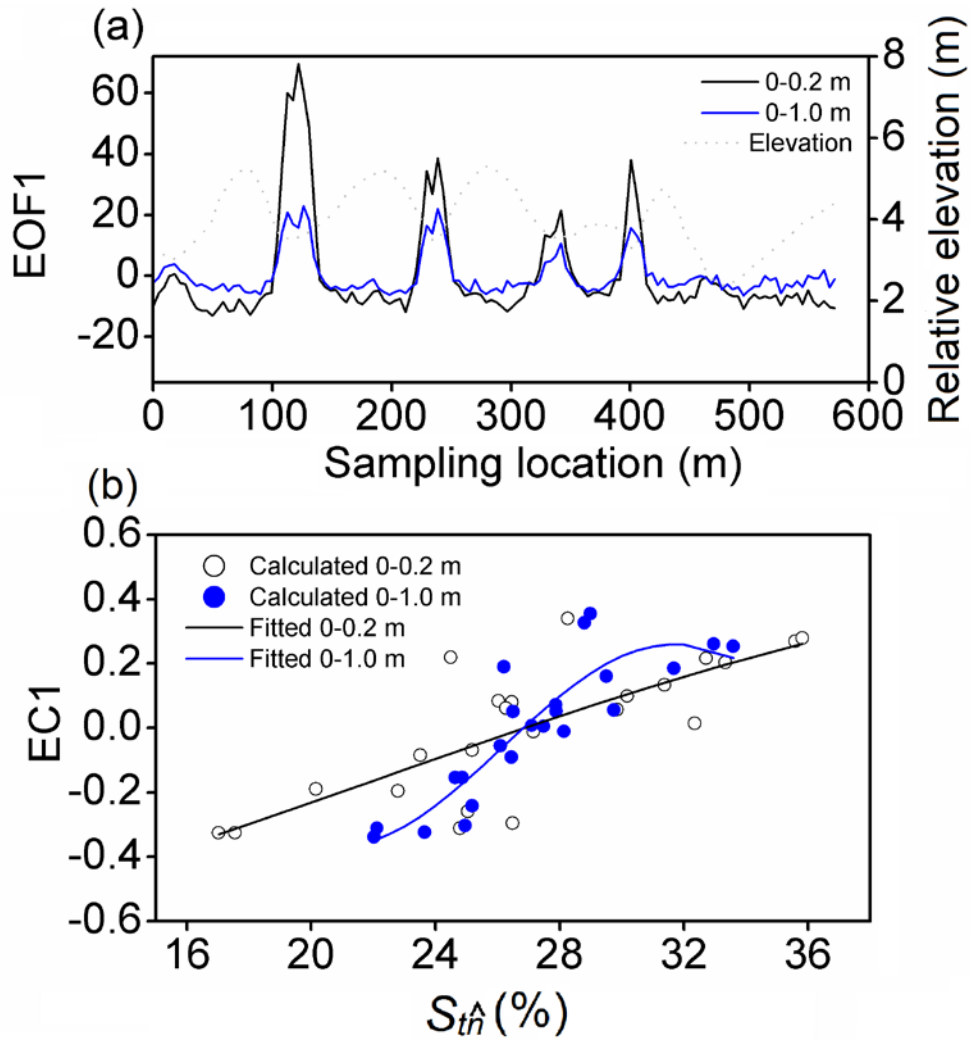


Fig. 6. (a) The EOF1 of the space-variant temporal anomaly R_{tn} and (b) relationships of associated EC1 versus spatial mean soil water content $S_{\hat{m}}$ fitted by the cosine function (Eq. 4).

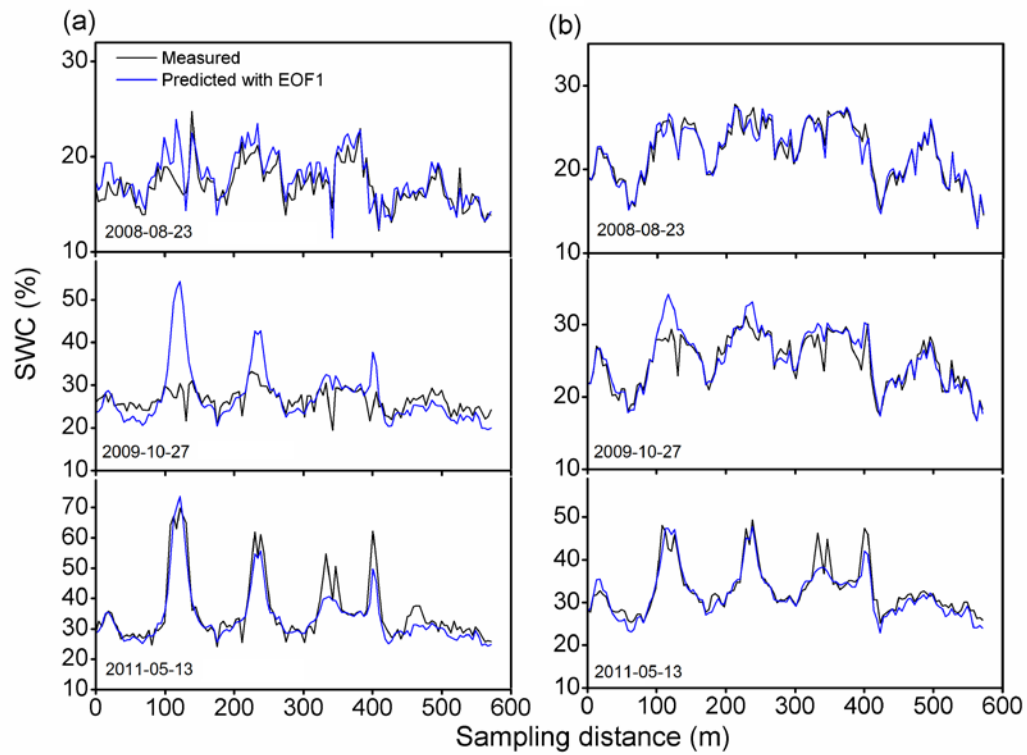


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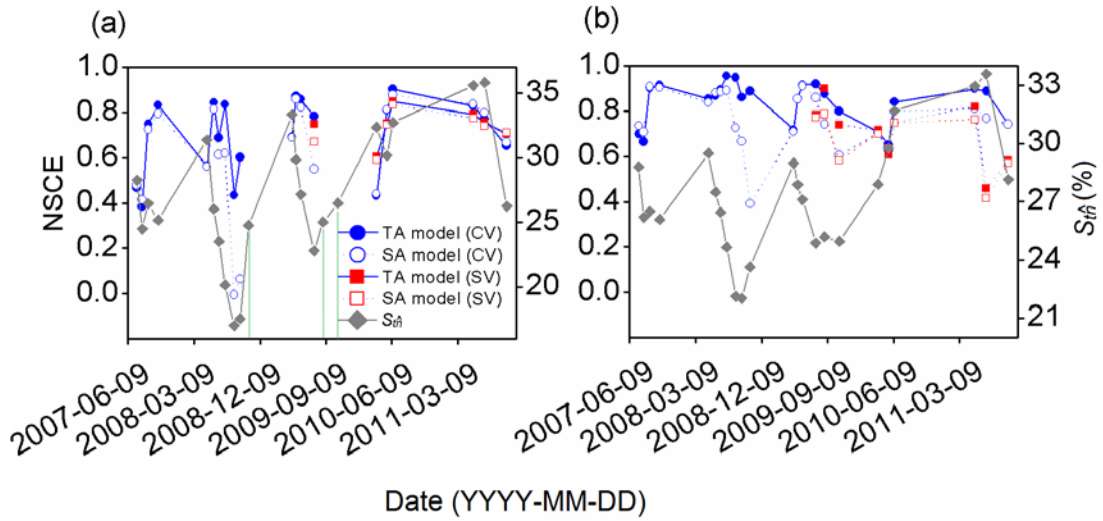


Fig. 8. The Nash-Sutcliffe coefficient of efficiency (NSCE) of soil water content estimation using the TA and SA models for (a) 0–0.2 and (b) 0–1.0 m for both cross validation (CV) and split sample validation (SV). At 0–0.2 m, three dates (October 22, 2008, August 27, 2009, and October 27, 2009) as indicated by green lines present negative NSCE values (-4.05, -1.83, and -3.81, respectively, for the CV on the three dates; -2.63 and -5.12, respectively, for the SV on the latter two dates). Spatial mean soil water content S_m on each measurement day is also shown.

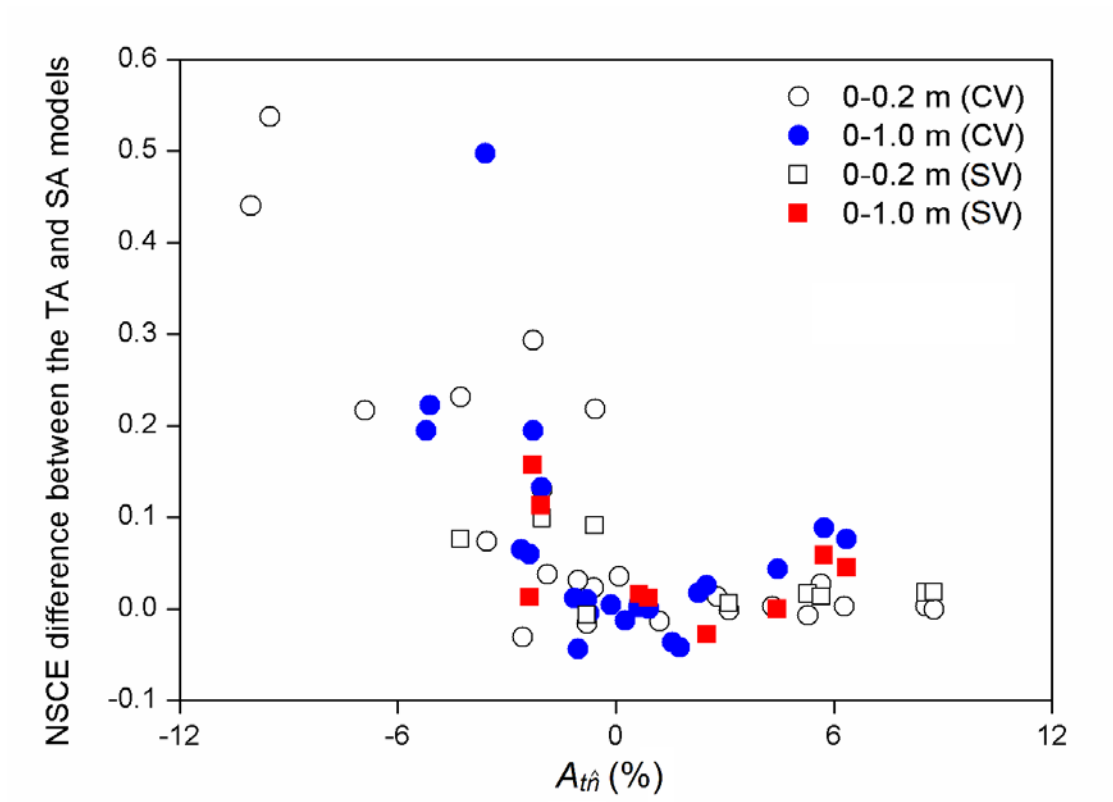


Fig. 9. Nash-Sutcliffe coefficient of efficiency (NSCE) difference between the TA and SA models in terms of soil water content estimation using both cross validation (CV) and split sample validation (SV) as a function of space-invariant temporal anomaly $A_{t\hat{n}}$ for (a) 0–0.2 and (b) 0–1.0 m.

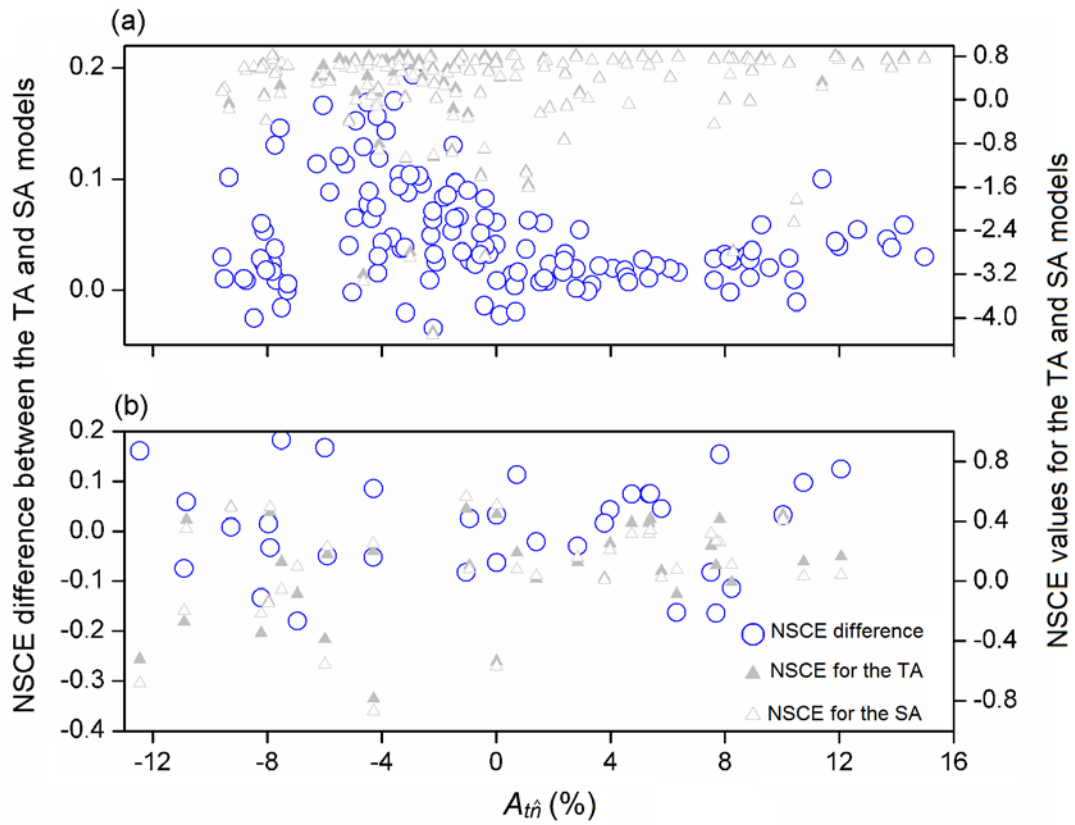


Fig. 10. Nash-Sutcliffe coefficient of efficiency (NSCE) difference between the TA and SA models in terms of soil water content estimation using cross validation as a function of space-invariant temporal anomaly $A_{t\hat{n}}$ for (a) 0–0.06 m of the Chinese Loess Plateau hillslope and (b) 0–0.15 m of the GENCAI network in Italy. The NSCE values for both models are also shown.