

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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6 **Abstract**

7 Soil water content (SWC) is crucial to rainfall-runoff response at the watershed scale.
8 A model was used to decompose the spatiotemporal SWC into a time-stable pattern
9 (i.e., temporal mean), a space-invariant temporal anomaly, and a space-variant
10 temporal anomaly. The space-variant temporal anomaly was further decomposed
11 using the empirical orthogonal function (EOF) for estimating spatially distributed
12 SWC. This model was compared to a previous model that decomposes the
13 spatiotemporal SWC into a spatial mean and a spatial anomaly, with the latter being
14 further decomposed using the EOF. These two models are termed temporal anomaly
15 (TA) model and spatial anomaly (SA) model, respectively. We aimed to test the
16 hypothesis that underlying (i.e., time-invariant) spatial patterns exist in the
17 space-variant temporal anomaly at the small watershed scale, and to examine the
18 advantages of the TA model over the SA model in terms of the estimation of spatially
19 distributed SWC. For this purpose, a dataset of near surface (0–0.2 m) and root zone
20 (0–1.0 m) SWC, at a small watershed scale in the Canadian prairies, was analyzed.
21 Results showed that underlying spatial patterns exist in the space-variant temporal

22 anomaly because of the permanent controls of “static” factors such as depth to the
23 CaCO_3 layer and organic carbon content. Combined with time stability analysis, the
24 TA model improved the estimation of spatially distributed SWC over the SA model,
25 especially for dry conditions. Further application of these two models demonstrated
26 that the TA model outperformed the SA model at a hillslope in the Chinese Loess
27 Plateau, but the performance of these two models in the GENCAI network (~250 km²)
28 in Italy was equivalent. The TA model has potential to construct a spatially distributed
29 SWC at small watershed scales from remote sensed SWC.

30 Keywords: Soil moisture; Soil water downscaling; Empirical orthogonal function;
31 Statistical models; Time stability

32 **1. Introduction**

33 Soil water content (SWC) of surface soils exerts a major influence on a series of
34 hydrological processes such as runoff and infiltration (Famiglietti et al., 1998;
35 Vereecken et al., 2007; She et al., 2013a). Soil water content in the root zone is, in
36 many cases, linked to vegetative growth (Wang et al., 2012; Ward et al., 2012; Jia and
37 Shao, 2013). Obtaining accurate information on the spatiotemporal SWC is crucial for
38 improving hydrological prediction and soil water management (Venkatesh et al., 2011;
39 Champagne et al., 2012; She et al., 2013b; Zhao et al., 2013). While remote sensing
40 has advanced SWC measurements of surface soils (<5 cm thick) at basin
41 (2,500–25,000 km²) and continental scales (Robinson et al., 2008), characterization of
42 spatially distributed SWC at small watershed (0.1–80 km²) scales still poses a

43 challenge. A method is needed for estimating spatially distributed SWC in the near
44 surface and root zone at watershed scales.

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

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

61 Recently, the spatiotemporal SWC was also decomposed into a temporal mean and
62 a temporal anomaly (Mittelbach and Seneviratne, 2012) (Fig. 1). Previous studies
63 indicated that the contribution of the temporal anomaly to the total spatial variance
64 was notable (Mittelbach and Seneviratne, 2012; Brocca et al., 2014; Rötzer et al.,

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

81 To our knowledge, the importance of the space-variant term of the temporal
82 anomaly and its physical meaning at small watershed scales is not well-known. Based
83 on previous studies (Perry and Niemann, 2007; Mittelbach and Seneviratne, 2012;
84 Vanderlinden et al., 2012), we assume soil water dynamics at watershed scales can be
85 decomposed into three components (Fig. 1): (1) time-stable pattern (i.e., temporal
86 mean, spatial forcing): the “static” factors such as soil and topography control the

87 pattern; (2) space-invariant temporal anomaly (temporal forcing): the “dynamic”
88 factors such as meteorological variables and vegetation change with time, and
89 therefore modify SWC in time, regardless of spatial locations; and (3) space-variant
90 temporal anomaly (interactions between spatial forcing and temporal forcing): this
91 term represents interactions between “static” and “dynamic” factors. For example,
92 SWC recharge introduced by a rainfall may be modified by topography through
93 runoff processes; SWC loss triggered by evapotranspiration may be regulated by
94 topography through solar radiation exposure.

95 The “static” factors may be persistent in the space-variant temporal anomaly, and
96 their impacts on the space-variant temporal anomaly likely change with time. Thus,
97 we hypothesize that some underlying (i.e., time-invariant) spatial patterns exist in the
98 space-variant temporal anomaly, and their impacts can be modulated by a time
99 coefficient, both of which can be obtained by the EOF method (Fig. 1). If the
100 hypothesis is true, the estimation of spatially distributed SWC utilizing the EOF
101 decomposition may outperform the one suggested by Perry and Niemann (2007). This
102 is because: (1) the spatial anomaly which was decomposed using the EOF in Perry
103 and Niemann (2007) lumped the time-stable pattern and space-variant temporal
104 anomaly together (Fig. 1); (2) the underlying spatial patterns in the spatial anomaly
105 may not fully capture both time-stable patterns and patterns in the space-variant
106 temporal anomaly due to the possible nonlinear relations between these two terms.

107 Therefore, the objectives were (1) to test the hypothesis that underlying spatial
108 patterns exist in the space-variant temporal anomaly at small watershed scales and (2)

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

122 **2. Materials and methods**

123 **2.1 Study area and data collection**

124 This study was conducted in the Canadian prairie pothole region at St. Denis
125 National Wildlife Area (52°12' N, 106°50' W) with an area of 3.6 km². This area has a
126 humid continental climate (Peel et al., 2007), and had a mean annual air temperature
127 of 1.9 °C and a mean annual precipitation of 402 mm during the study period (Fig. 2).
128 A variety of depressions, knolls, and knobs result in a sequence of undulating slopes
129 (Biswas et al., 2011). The elevation varies from 554.8 to 557.5 m. The soils are

130 dominated by clay loam textured Mollisols (Soil Survey Staff, 2010) and covered by
131 mixed grass, i.e., smooth brome grass (*Bromus inermis*) and alfalfa (*Medicago sativa*
132 L.). The near surface soil porosity ranges from 38% (knolls) to 70% (depressions).
133 Calcium carbonates (CaCO_3) derived mostly from fragments of limestone rocks are
134 common in the Canadian Prairies. The CaCO_3 is dissolved by the slightly acidic
135 rainwater moving through the upper horizons and deposited to lower horizons. The
136 heterogeneous amount of infiltrated water resulted in a varying depth of CaCO_3 layer
137 ranging from almost 0 m in the knolls to 2.1 m in the depressions. A 576 m long
138 sampling transect with 128 sampling locations spaced at 4.5 m intervals was
139 established over several rounded knolls and depressions. At each location, a time
140 domain reflectometry probe was used to measure SWC of the near surface soil (0–0.2
141 m), and a neutron probe was used to collect SWC measurements at 0.2 m intervals
142 between a depth of 0.2 and 1.0 m. The SWC was measured on a volumetric basis and
143 expressed as a percentage (%) volume of water per unit soil volume. The SWC of the
144 root zone was calculated by averaging the SWC of 0–0.2, 0.2–0.4, 0.4–0.6, 0.6–0.8,
145 and 0.8–1.0 m. Soil water content was measured on 23 dates from July 17, 2007 to
146 September 29, 2011. The SWC dataset was collected in all seasons except winter, and
147 accurately portrays the variations in soil water conditions in the study area. In addition
148 to the SWC dataset, the soil, vegetative, and topographical properties were obtained at
149 each sampling location. These properties included soil particle components (clay, silt,
150 and sand contents), bulk density, soil organic carbon (SOC) content for the surface
151 layer, A horizon depth, C horizon depth, depth to the CaCO_3 layer, leaf area index,

152 elevation, $\cos(\text{aspect})$, slope, curvature, gradient, upslope length, solar radiation,
153 specific contributing area, convergence index, wetness index, and flow connectivity.
154 Detailed information on the measurements can be found in Biswas et al. (2012).

155 **2.2 Statistical models for decomposing soil water content**

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

167 **2.2.1 The SA model**

168 Perry and Niemann (2007) expressed SWC at location n and time t (S_{tn}) as (Fig.
169 1):

$$170 \quad S_{tn} = S_{t\hat{n}} + Z_{tn}, \quad (1)$$

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

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

175 water balance models, and in situ soil water measurement at a representative (or
 176 time-stable) location. The in situ soil water measurement method was selected
 177 because the representative location can be easily determined with prior SWC datasets.
 178 By measuring SWC only at the most time-stable location (s) and future time t (S_{ts}),
 179 $S_{\hat{m}}$ can be estimated using (Grayson and Western, 1998):

$$180 \quad S_{\hat{m}} = \frac{S_{ts}}{1 + \delta_{ts}} \quad , \quad (2)$$

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

184 Spatial anomaly (Z_m) can be reconstructed by the sum of the product of
 185 time-invariant spatial structures (EOFs) and temporally varying coefficients (ECs)
 186 using the EOF method (Perry and Niemann, 2007; Joshi and Mohanty, 2010;
 187 Vanderlinden et al., 2012). The ECs correspond to the eigenvectors of the matrix of
 188 spatial covariance of the Z_m , and the EOFs are obtained by projecting the Z_m onto
 189 the matrix ECs as: EOFs = Z_m ECs. The number of EOF (or EC) series equals the
 190 number of sampling dates. Each EOF series corresponds to one value at each location,
 191 and each EC series has one value at each measurement time. Each EOF is chosen to
 192 be orthogonal to other EOFs, and the lower-order EOFs account for as much variance
 193 as possible. The sum of variances of all EOFs equals the sum of variances of Z_m
 194 from all measurement times.

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

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

$$200 \quad Z_{tm} = \sum \text{EOF}^{sig} \times (\text{EC}^{sig})^T, \quad (3)$$

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

$$206 \quad \text{EC}_t = a + b \cos\left(\frac{2\pi}{c} S_{\hat{m}} - d\right), \quad (4)$$

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

211 **2.2.2 The TA model**

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

$$214 \quad S_{tm} = M_{\hat{m}} + A_{tm}, \quad (5)$$

215 where $M_{\hat{m}}$ is the time-stable pattern (spatial forcing) controlled by “static” factors
 216 such as soil properties and topography; A_{tm} refers to the temporal anomaly (lumped
 217 temporal forcing and interactions). The variance of SWC ($\sigma_{\hat{n}}^2(S_{tm})$) is the sum of
 218 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

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

$$220 \quad \sigma_{\hat{n}}^2(S_m) = \sigma_{\hat{n}}^2(M_{\hat{m}}) + 2\text{cov}(M_{\hat{m}}, A_m) + \sigma_{\hat{n}}^2(A_m). \quad (6)$$

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

$$232 \quad S_m = M_{\hat{m}} + A_{\hat{m}} + R_m. \quad (7)$$

233 The temporal trends of $A_{\hat{m}}$ in Eq. (7) and $S_{\hat{m}}$ in Eq. (1) are the same as both
 234 represent temporal forcing. Because the $A_{\hat{m}}$ is space-invariant and orthogonal to the
 235 $M_{\hat{m}}$ and R_m in a space, $\sigma_{\hat{n}}^2(S_m)$ in Eq. (6) can also be written as:

$$236 \quad \sigma_{\hat{n}}^2(S_m) = \sigma_{\hat{n}}^2(M_{\hat{m}}) + 2\text{cov}(M_{\hat{m}}, R_m) + \sigma_{\hat{n}}^2(R_m), \quad (8)$$

237 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
 238 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
 239 $\sigma_{\hat{n}}^2(R_m)$ equals $\sigma_{\hat{n}}^2(A_m)$. The percent (%) contributions of $\sigma_{\hat{n}}^2(M_{\hat{m}})$,
 240 $2\text{cov}(M_{\hat{m}}, R_m)$, and $\sigma_{\hat{n}}^2(R_m)$ to the $\sigma_{\hat{n}}^2(S_m)$ are calculated. The $\text{cov}(M_{\hat{m}}, R_m)$

241 can be negative at some conditions, for example, when the depressions correspond to
 242 greater $M_{\hat{m}}$ and more negative R_m values in the discharge periods. This resulted
 243 in percentage contributions of $\sigma_{\hat{m}}^2(M_{\hat{m}})$ and $\sigma_{\hat{m}}^2(R_m) > 100\%$ and percentage
 244 contributions of $2\text{cov}(M_{\hat{m}}, R_m) < 0\%$ (Mittelbach and Seneviratne, 2012; Brocca et
 245 al., 2014; Rötzer et al., 2015). If R_m is zero at any time or location, there are no
 246 interactions between spatial forcing and temporal forcing, $\sigma_{\hat{m}}^2(S_m)$ and the spatial
 247 trends of SWC are consistent over time. Therefore, R_m is directly responsible for
 248 temporal change in the spatial variability of SWC.

249 If some underlying spatial patterns exist in R_m , R_m can be reconstructed by the
 250 sum of the product of time-invariant spatial structures (EOFs) and time-dependent
 251 coefficients (ECs) using the EOF method. Note that the number of EOF (or EC) series
 252 also equals the number of sampling dates.

253 For estimation of spatially distributed SWC, R_m is estimated by the same method
 254 as Z_m using Eq. (3). The $M_{\hat{m}}$ is estimated with prior measurements by:

$$255 \quad M_{\hat{m}} = \frac{1}{m} \sum_{j=1}^m S_m, \quad (9)$$

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

$$257 \quad A_{\hat{m}} = S_{\hat{m}} - M_{\hat{m}}, \quad (10)$$

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

260 The Pearson correlation coefficient (R) is used to explore the linear relationships
 261 between various spatial components in the two models (i.e., EOF1 of the Z_m in the
 262 SA model, $M_{\hat{m}}$, and EOF1 of the R_m in the TA model) and environmental factors

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

266 **2.3 Validation and performance parameter**

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

$$269 \quad AICc = 2k + n \ln(RSS / n) + 2k(k + 1) / (n - k - 1), \quad (11)$$

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

272 Both cross validation and external validation are used to estimate SWC distribution
273 with both models. For the cross validation, an iterative removal of 1 of the 23 dates is
274 made for model development, and the SWC along the transect corresponding to the
275 removed date is estimated iteratively. For the external validation, SWC from 14 dates
276 of the first two years (from July 17, 2007 to May 27, 2009) is used for model
277 development, and the SWC distribution of 9 dates in the second two years (from July
278 21, 2009 to September 29, 2011) is estimated.

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

$$281 \quad NSCE = 1 - \frac{\sigma_{\varepsilon}^2}{\sigma_{measure}^2}, \quad (12)$$

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

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

286 Many factors may affect the relative performance of spatially distributed SWC
287 estimation between the TA model and the SA model. First, the degree of
288 outperformance of the TA model over the SA model may depend on the amount of
289 R_{tn} variance considered in the TA model. On one hand, the two models are identical
290 if variance of R_{tn} is close to zero or there are negligible interactions between the
291 spatial and temporal components (Fig. 1). On the other hand, if no underlying spatial
292 patterns exist in the R_{tn} or the underlying spatial patterns contributed little to the
293 total variance of the R_{tn} , the outperformance will also be very limited. Therefore, the
294 greater the variance of R_{tn} considered in the TA model, the more likely the TA
295 model can outperform the SA model. Second, the way of EOF decomposition may
296 also affect the relative performance. In the SA model, EOF decomposition is
297 performed on lumped time-stable patterns ($M_{\hat{tn}}$) and space-variant temporal anomaly
298 (R_{tn}). In the TA model, however, EOF decomposition is made only on the R_{tn} . In
299 theory, the two models will be identical if the $M_{\hat{tn}}$ and the first underlying spatial
300 pattern (i.e., EOF1) of the R_{tn} were perfectly correlated. If a nonlinear relationship
301 exists between them, lumping the $M_{\hat{tn}}$ and R_{tn} together, as in the SA model,
302 would weaken the model performance as compared to the TA model. From this aspect,
303 the greater deviation from a linear relationship between the $M_{\hat{tn}}$ and EOF1 of the
304 R_{tn} , may lead to a greater outperformance of the TA model over the SA model.
305 Finally, the performances of both models rely on the estimation accuracy of the EC_t
306 which depends on both goodness of fit of the cosine function (i.e., Eq. 4) and

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

310 **3. Results**

311 **3.1 Components of SWC and their controls**

312 **3.1.1 Spatial mean (S_{in}) and spatial anomaly (Z_{in})**

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

321 The spatial patterns of spatial anomaly (Z_{in}) were similar to those of original SWC
322 patterns. The values of Z_{in} in wet periods (e.g., May 13, 2011) were much greater
323 than in dry periods (e.g., August 23, 2008) in depressions (e.g., at a distance of 123
324 and 250 m); at other locations, however, the spatial anomaly was slightly less in wet
325 periods than in dry periods for both soil layers. Moreover, the spatial anomaly in
326 depressions during the wet periods was much greater in the near surface than in the
327 root zone.

328 When SWCs of all 23 dates were used for model development, only EOF1 was
 329 statistically significant (Fig. 4a), which accounted for 84.3% (0–0.2 m) and 86.5%
 330 (0–1.0 m) of the variances in the Z_{in} . Correlation analysis indicated that the spatial
 331 pattern of EOF1 in the Z_{in} was identical to the time-stable patterns ($M_{\hat{in}}$) in the TA
 332 model ($R=1.0$). The controls of EOF1 was therefore the same as those of $M_{\hat{in}}$, and
 333 will be discussed later. The relationship between associated EC1 and $S_{\hat{in}}$ can be
 334 fitted well by the cosine function ($R^2=0.73$ at both the near surface and root zone) (Fig.
 335 4b).

336 **3.1.2 Time-stable pattern ($M_{\hat{in}}$), space-invariant temporal anomaly ($A_{\hat{in}}$), and**
 337 **space-variant temporal anomaly (R_{in})**

338 Figure 3b displays the three components in the TA model. The first component
 339 $M_{\hat{in}}$ fluctuated along the transect, with high values in depressions and low values on
 340 knolls; the $M_{\hat{in}}$ also had greater spatial variability in the near surface (variance
 341 $=36.7\%^2$) than in the root zone (variance $=19.5\%^2$). For both soil layers, SOC, depth to
 342 the CaCO_3 layer, sand content, and wetness index are the dominant factors of $M_{\hat{in}}$;
 343 they together explained 74.5% (near surface) and 75.6% (root zone) of the variances
 344 in the $M_{\hat{in}}$ (Table 1). In addition, the temporal trend of $A_{\hat{in}}$ was the same as that of
 345 $S_{\hat{in}}$ in the SA model (Fig. 3a) as both represent temporal forcing.

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

350 corresponded to more positive R_{tm} during the wet periods and more negative R_{tm}
351 during the dry periods. This implies that topographically lower locations gained more
352 water during recharge and lost more water during discharge due to the interactions of
353 spatial and temporal forcing. Furthermore, the absolute values of R_{tm} were generally
354 greater in the near surface than the root zone, indicating a greater space-variant
355 temporal anomaly for shallower depths.

356 The SWC variances and associated components (Eq. 8) also varied with time (Fig.
357 5). Often, wetter conditions corresponded to greater $\sigma_{\hat{n}}^2(S_m)$, as further indicated by
358 moderate correlation between $\sigma_{\hat{n}}^2(S_m)$ and $S_{\hat{m}}$ (R^2 of 0.51 and 0.38 for the near
359 surface and the root zone, respectively). This was in agreement with others
360 (Gómez-Plaza et al., 2001; Martínez-Fernández and Ceballos, 2003; Hu et al., 2011).
361 Furthermore, there were greater $\sigma_{\hat{n}}^2(S_m)$ values at near surface than in the root zone,
362 indicating greater variability of SWC in the near surface.

363 The time-invariant $\sigma_{\hat{n}}^2(M_{\hat{m}})$ contributed to the $\sigma_{\hat{n}}^2(S_m)$ with percentages
364 ranging from 25 to 795% for the near surface and from 40 to 174% for the root zone
365 (Fig. 5). The $\sigma_{\hat{n}}^2(M_{\hat{m}})$ exceeded the $\sigma_{\hat{n}}^2(S_m)$ mainly under dry conditions, such as
366 July–October in 2008 and 2009. This excess was offset by the $\sigma_{\hat{n}}^2(S_m)$ and
367 $2\text{cov}(M_{\hat{m}}, R_m)$, with the latter contributing negatively to the $\sigma_{\hat{n}}^2(S_m)$ with mean
368 percentages of 210% for the near surface and 17% for the root zone. In the dry period,
369 the negative contribution from $2\text{cov}(M_{\hat{m}}, R_m)$ was up to 1327% for the near surface
370 and 122% for the root zone. These values are comparable to those in Mittelbach and
371 Seneviratne (2012) and Brocca et al. (2014).

372 The $\sigma_{\hat{n}}^2(R_m)$ contributed less than other components (Fig. 5). The percentages of
373 $\sigma_{\hat{n}}^2(R_m)$ ranged from 11 to 632% (arithmetic average of 118%) for the near surface
374 and from 6 to 48% (arithmetic average of 19%) for the root zone; $\sigma_{\hat{n}}^2(R_m)$ tended to
375 contribute more in drier periods. This indicates that the space-variant temporal
376 anomaly cannot be ignored, particularly in dry conditions. Furthermore, the
377 contribution of $\sigma_{\hat{n}}^2(R_m)$ was greater in the near surface than in the root zone,
378 confirming stronger temporal dynamics of soil water at the near surface. Compared
379 with larger scale studies (Mittelbach and Seneviratne, 2012; Brocca et al., 2014),
380 $\sigma_{\hat{n}}^2(R_m)$ of the near surface contributed more to $\sigma_{\hat{n}}^2(S_m)$, with a mean percentage
381 contribution of 118%, versus 9–68% in the other, larger scale studies. This indicates
382 that interactions between spatial and temporal forcing were stronger, resulting in
383 relatively more intensive temporal dynamics of soil water in our study area than at
384 larger scales.

385 Three significant EOFs of R_m for both soil layers were identified when SWC of
386 all 23 dates were used for model development. The first three EOFs explained 61.1,
387 13.4, and 8.1% respectively, of the total R_m variance for the near surface, and 44.3,
388 20.2, and 12.4%, respectively, of the total R_m variance in the root zone. Therefore,
389 our hypothesis that underlying spatial patterns exist in the R_m was accepted. Due to
390 the negligible contribution of EOF2 and EOF3 to the estimation of spatially
391 distributed SWC, only EOF1 is shown in Fig. 6a. The associated EC1 changed with
392 soil water conditions ($S_{\hat{m}}$) (Fig. 6b). When SWC was close to average levels, the EC1
393 was close to 0, resulting in negligible R_m . This was in accordance with Mittelbach

394 and Seneviratne (2012) and Brocca et al. (2014), who showed that the spatial variance
395 of the temporal anomaly was the smallest when water contents were close to average
396 levels. The cosine function (Eq. 4) explained a large amount of the variances in EC1
397 for both soil layers ($R^2=0.76$ at the near surface and 0.88 in the root zone).

398 The contribution of EOF1 to the space-variant temporal anomaly can be examined
399 through the product of the EOF1 and the associated EC1. The EC1 values tended to
400 be positive during wet periods and negative during dry periods (Fig. 6b); more
401 positive EOF1 values were usually observed at locations with greater M_{in} values
402 (Figs. 3b and 6a). Therefore, the product of EOF1 and EC1 led to greater temporal
403 SWC dynamics at wetter locations of both layers in both the wet and dry periods.

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

410 **3.2 Estimation of spatially distributed SWC**

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

416 3.2.1 The TA model

417 The R_m terms and associated EOFs differed slightly with each validation. The
418 number of significant EOFs varied between one (accounting for 60% of the total cases)
419 and three for both soil layers. A paired samples T-test indicated that more EOFs did
420 not result in a significant increase of NSCE in the estimation of spatially distributed
421 SWC for both validation methods, because AICc values increased greatly with the
422 increasing number of parameters resulting from more EOFs (data not shown). This
423 indicates that higher-order EOFs, even if they are statistically significant, are
424 negligible for SWC prediction. Therefore, SWC distribution was estimated with
425 EOF1 only.

426 Estimated SWCs generally approximated those measured at different soil water
427 conditions during the cross validation (Fig. 7). However, on October 27, 2009, there
428 were unsatisfactory estimates at the 100–140 and 220–225 m locations near the
429 surface. Unsatisfactory NSCE values of -4.05, -1.83, and -3.81 were obtained in the
430 near surface in only three of the 23 dates, which were all in the fall (October 22, 2008,
431 August 27, 2009, and October 27, 2009, respectively). The poor performance obtained
432 with the TA model on those dates was a result of overestimation in depressions, where
433 strong evapotranspiration and deep drainage resulted in a much lower SWC than in
434 the spring. These dates also corresponded to a high percentage of contribution of
435 $\sigma_{\hat{n}}^2(R_m)$ to the $\sigma_{\hat{n}}^2(S_m)$ (203–439%). For August 23 and September 17 in 2008,
436 which were in dry periods, $\sigma_{\hat{n}}^2(R_m)$ of the near surface also contributed highly to the
437 $\sigma_{\hat{n}}^2(S_m)$ (580 and 630%). Because a fair amount of $\sigma_{\hat{n}}^2(R_m)$ was accounted for

438 with the TA model, the TA model performed satisfactorily (NSCE of 0.43 and 0.60).
439 For the remaining 20 dates, the resulting NSCE value ranged from 0.38 to 0.90 in the
440 near surface and from 0.65 to 0.96 in the root zone (Fig. 8). This suggests that the TA
441 model was generally satisfactory, with better performance in the root zone than in the
442 near surface.

443 During the external validation, the TA model resulted in SWC estimations with
444 NSCE values ranging from 0.61 to 0.85 near the surface and from 0.32 to 0.92 in the
445 root zone, with exception of two days (August 27, 2009 and October 27, 2009 with
446 NSCE values of -2.63 and -5.12, respectively) at 0–0.2 m (Fig. 8). This suggested that
447 the TA model performed well in estimating spatially distributed SWC patterns except
448 on August 27, 2009 and October 27, 2009 at 0–0.2 m. The estimation in the root zone
449 was also generally better than in the near surface.

450 **3.2.2 Comparison with the SA model**

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

460 The difference in NSCE values between the TA and SA models for both validations
461 are presented in Fig. 9. Generally, the difference decreased as $A_{\hat{m}}$ increased, and
462 then slightly increased with a further increase in $A_{\hat{m}}$. A paired samples T-test
463 indicated that the NSCE values of the TA model were significantly ($P<0.05$) greater
464 than those of the SA model for both soil layers, irrespective of validation methods.
465 This indicates that the TA model outperformed the SA model, particularly in dry
466 conditions. This was because when the soil was dry, there was a high contribution of
467 $\sigma_{\hat{n}}^2(R_m)$, and thus strong variability in the space-variant temporal anomaly.

468 **3.3 Further application at other two sites with different scales**

469 **3.3.1 A hillslope in the Chinese Loess Plateau**

470 Along a hillslope of 100 m in length in the Chinese Loess Plateau, SWC of 0–0.06
471 m was measured 136 times from June 25, 2007 to August 30, 2008 by a Delta-T
472 Devices Theta probe (ML2x) at 51 locations (Hu et al., 2011). The hillslope was
473 covered by *Stipa bungeana* Trin. and *Medicago sativa* L. in sandy loam and silt loam
474 soils. On average, the $\sigma_{\hat{n}}^2(M_{\hat{m}})$, $\sigma_{\hat{n}}^2(R_m)$, and $2\text{cov}(M_{\hat{m}}, R_m)$ contributed 53, 74
475 and -27% to the $\sigma_{\hat{n}}^2(S_m)$, indicating that both time-stable pattern and temporal
476 anomalies were the main contributors to the $\sigma_{\hat{n}}^2(S_m)$. The EOF analysis showed that
477 only the EOF1 was statistically significant for both the R_m and Z_m , and the EOF1
478 explained 23% and 47% of the total variances of R_m and Z_m , respectively. This
479 illustrated that underlying spatial patterns exist in the R_m on the hillslope. Cross
480 validation was used to estimate the spatially distributed SWC along the hillslope. The
481 results showed that the NSCE varied from -4.25 to 0.83 (TA model) and from -4.30 to

482 0.81 (SA model), with a mean value of 0.25 and 0.18, respectively. A paired samples
483 T-test showed that the NSCE values for the TA model were significantly ($P<0.05$)
484 greater than those for the SA model, indicating that the TA model outperformed the
485 SA model. As Fig. 10a shows, the outperformance was greater when SWC deviated
486 from intermediate conditions, especially for dry conditions, which was similar to the
487 Canadian site.

488 3.3.2 The GENCAI network in Italy

489 In the GENCAI network ($\sim 250 \text{ km}^2$) in Italy, SWC of 0–0.15 m was measured by a
490 TDR probe at 46 locations, 34 times from February to December in 2009 (Brocca et
491 al., 2012, 2013). The GENCAI area was dominated by grassland with a flat
492 topography, in silty clay soils. The $\sigma_{\hat{n}}^2(M_{\hat{m}})$, $\sigma_{\hat{n}}^2(R_m)$, and $2\text{cov}(M_{\hat{m}}, R_m)$
493 contributed 38, 68, and -7% to the $\sigma_{\hat{n}}^2(S_m)$ (Brocca et al., 2014), indicating the
494 dominant contribution of temporal anomalies on SWC variability. The first three
495 EOFs of the R_m explained 19, 16, and 8% of the total $\sigma_{\hat{n}}^2(R_m)$, and no EOFs were
496 statistically significant, indicating that no underlying spatial patterns exist in the R_m .
497 The EOF1 of the Z_m was significant and accounted for 37% of the variances in the
498 Z_m . Although the EOF1 of the R_m was not significant, it was considered in the TA
499 model for estimating spatially distributed SWC. The cross validation indicates that the
500 NSCE varied from -0.79 to 0.50 (TA model) and from -0.87 to 0.56 (SA model), with
501 mean values of 0.09 and 0.08, respectively. The SWC estimation based on these two
502 models was not satisfactory except for a few days. As Fig. 10b shows, the differences
503 in NSCE values between the two models were scattered around 0. A paired samples

504 T-test showed that the NSCE values between the TA model and the SA model were
505 not significant ($P<0.05$), indicating no differences in estimating spatially distributed
506 SWC between these two models.

507 **4 Discussion**

508 **4.1 Controls of the $M_{\hat{m}}$ and R_m**

509 The R_m played an important role in the temporal change in spatial patterns of the
510 SWC. The underlying spatial patterns and physical meaning in the R_m were
511 examined in our study for the first time. Although three significant EOFs of the R_m
512 existed in some cases, only EOF1 rather than higher-order EOFs of the R_m should
513 be considered for the spatially distributed SWC estimation. Among many factors
514 influencing the EOF1 of the R_m , depth to the CaCO_3 layer followed by the SOC,
515 were the most important factors. Depressions have deeper CaCO_3 layers than knolls,
516 and the shallow CaCO_3 layer on knolls limited water infiltration during rainfall or
517 snowmelt, resulting in less water recharge on knolls than in depressions. The depth to
518 CaCO_3 layer and SOC were negatively correlated with elevation ($R=-0.54$, $P<0.01$).
519 Therefore, the influence of depth to CaCO_3 layer and SOC partially reflected the role
520 of topography in driving snowmelt runoff along slopes in the spring, which
521 contributes to increasing water recharge in depressions. Locations with greater SOC
522 usually corresponded to vegetation with a larger leaf area index ($R=0.23$, $P<0.05$),
523 which would also result in higher evapotranspiration and more water loss during
524 discharge periods.

525 As Table 1 shows, both the depth to the CaCO_3 layer and SOC controlled the $M_{\hat{m}}$.
526 This was because deeper CaCO_3 layers and higher SOC were observed in depressions
527 where soils were usually wetter in most of the year because of the snowmelt runoff in
528 the spring and rainfall runoff in the summer and autumn (van der Kamp et al., 2003).
529 Therefore, the roles of soil and topography were two-fold: On one hand, they were
530 highly correlated with the time-stable patterns and thus the time stability of SWC
531 (Gómez-Plaza et al., 2000; Mohanty and Skaggs, 2001; Grant et al., 2004); On the
532 other hand, soil and topography, interplaying with temporal forcing, triggered
533 local-specific soil water change and destroyed time stability of SWC. Their roles in
534 protecting time stability persisted, but their roles in destroying time stability varied
535 with time. Greater $\sigma_n^2(R_m)$ implies greater contribution of these factors in soil water
536 dynamics, resulting in less time stability of SWC.

537 **4.2 Model performance for spatially distributed SWC estimation**

538 The outperformance of the TA model for estimating spatial SWC at the Canadian
539 site and Chinese site can be partly explained by the high contribution percentages
540 (average of 19–118%) of the $\sigma_n^2(R_m)$ to the total variance. When SWC is close to
541 average levels, R_m is also close to zero, resulting in negligible variance contribution
542 from R_m to the total variance. In this case, the soil water patterns are stable, the SA
543 model performs well, and there will be little differences between these two models.
544 As is well known, the spatial patterns in soil water content are inherently time
545 unstable. For example, when evapotranspiration becomes the dominant process at the
546 small watershed scale, more water will be lost in depressions due to the denser

547 vegetation than on knolls (Millar, 1971; Biswas et al., 2012), effectively diminishing
548 the spatial patterns and increasing temporal instability. In this case, the $\sigma_n^2(R_m)$
549 contributes more to the total variance (e.g., high up to 632%) and the TA model may
550 outperform the SA model. This explained why the outperformance of the TA model
551 was more obvious in the dry conditions. For the GENCAI network in Italy, although
552 the $\sigma_n^2(R_m)$ contributed 68% of the total variance, the performance of the TA model
553 was identical to the SA model. This was because there were no underlying spatial
554 patterns in the R_m . Similarly, because the first underlying spatial pattern (i.e., EOF1)
555 explained greater percentages of the $\sigma_n^2(R_m)$ at the Canadian site (44–61%) than the
556 Chinese site (23%), the outperformance of the TA model over the SA model was more
557 obvious at the former site (Fig. 9 and 10a). Therefore, the TA model is advantageous
558 only if the contribution of $\sigma_n^2(R_m)$ to the total variance is substantial and underlying
559 spatial patterns exist in the R_m .

560 The existence of underlying spatial patterns in the R_m is related to the controlling
561 factors, which may be scale-specific. At small scales, “static” factors such as the depth
562 to the CaCO₃ layer and SOC at the Canadian site may affect not only the time-stable
563 patterns but also the R_m . The persistent influence of “static” factors on the R_m
564 resulted in significant underlying spatial patterns in the R_m . Thus, the TA model
565 outperformed the SA model at the small scales. At large scales such as the basin scale
566 or greater, time-stable patterns may be controlled by, in addition to soil and
567 topography (Mittelbach and Seneviratne, 2012), the climate gradient (Sherratt and
568 Wheater, 1984); at those scales, R_m is more likely to be controlled by the

569 meteorological anomaly (i.e., spatially random variation) (Walsh and Mostek, 1980),
570 and the effects of soil and topography may be reduced. Consequently, spatial patterns
571 in the R_{tm} may be weakened and the TA model may have no advantages over the SA
572 model such as for the Italian site.

573 The $M_{\hat{m}}$ and the underlying spatial patterns (EOF1) in the R_{tm} were controlled
574 by the same spatial forcing (e.g., depth to CaCO_3 layer and SOC) at the Canadian site
575 (Table 1), and they were correlated with an R^2 of 0.83 for the near surface and 0.42 for
576 the root zone. Although the relationships between $M_{\hat{m}}$ and R_{tm} were strong, they
577 were not strictly linear, suggesting that $M_{\hat{m}}$ and R_{tm} were affected differently by
578 these factors. Therefore, the nonlinear relationship between $M_{\hat{m}}$ and R_{tm} partially
579 contributed to the outperformance of the TA model over the SA model.

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

585 Therefore, the outperformance of the TA model over the SA model depends on
586 counterbalance among the variance of R_{tm} explained in the TA model, the linear
587 correlation between the $M_{\hat{m}}$ and EOF1 of the R_{tm} , and the goodness of fit for the
588 $S_{\hat{m}}$ and EC1 relationship. For example, the variance of EOF1 in the R_{tm} for the near
589 surface (i.e., 264%²) was much greater than that for the root zone (i.e., 43%²).
590 However, $M_{\hat{m}}$ and underlying spatial patterns (EOF1) in the R_{tm} in the root zone

591 deviated more from a linear relationship, and the reduced scatter in the $S_{\hat{m}}$ and EC1
592 relationship in the TA model was more obviously in the root zone than in the near
593 surface. As a result, the outperformance of the TA model was comparable between the
594 near surface and root zone at the Canadian site (Fig. 9).

595 In the real world, the relations between the $M_{\hat{m}}$ and underlying spatial patterns in
596 the R_m may rarely be perfectly linear. Therefore, when underlying spatial patterns
597 exist in the R_m and the R_m has substantial variances, the TA model is preferable
598 to the SA model for the estimation of spatially distributed SWC. Because the TA
599 model was not worse than the SA model for the whole range of SWC, the TA model is
600 suggested for the estimation of spatially distributed SWC at different soil water
601 conditions.

602 Previous studies on SWC decomposition mainly focus on near surface layers
603 (Jawson and Niemann, 2007; Perry and Niemann, 2007, 2008; Joshi and Mohanty,
604 2010; Korres et al., 2010; Busch et al., 2012). This study decomposed spatiotemporal
605 SWC using the TA model for both the near surface and the root zone. The results
606 showed that the estimation of spatially distributed SWC at small watershed scales was
607 improved by the TA method that considers the R_m . Because of the stronger time
608 stability of SWC in deeper soil layers (Biswas and Si, 2011), SWC evaluation in
609 thicker soil layers was more accurate than in shallow soil layers. This is particularly
610 important because SWC data for deeper soil layers in a watershed is more difficult to
611 collect than that of surface soil.

612 5 Conclusions

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

626 This study showed that outperformance of the TA model over the SA model is
627 possible when $\sigma_{\hat{n}}^2(R_m)$ contributes substantial variance to the total variance of SWC,
628 and significant spatial patterns (or EOFs) exist in the R_m . Further application of the
629 TA model for the estimation of spatially distributed SWC at different scales and
630 hydrological backgrounds is recommended. If the TA model parameters (i.e., $M_{\hat{m}}$,
631 EOF1 of the R_m , and relationship between EC and $S_{\hat{m}}$) are obtained from historical
632 SWC datasets, a detailed spatially distributed SWC of near surface soil at watershed
633 scales can be constructed from remote sensed SWC. Note that both models rely on

634 previous SWC measurements for model parameters. Therefore, the future study
635 should be directed to estimate spatially distributed SWC in un-gauged watersheds
636 based on the estimation of the model parameters using pedotransfer functions. Since
637 the TA model needs one more spatial parameter (i.e., M_{in}) than the SA model, the
638 advantage of the TA model may be weakened. Nevertheless, the TA model may be
639 preferred if it estimates spatial SWC much better than the SA model such as under dry
640 conditions. The codes for decomposing SWC with the SA and TA models and related
641 EOF analysis were written in Matlab and are freely available from the authors upon
642 request.

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790 **Figure captions**

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

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

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

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

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

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

807 **Figure 7.** Estimated soil water content (SWC) versus measured SWC for three dates
808 at different soil water conditions (August 23, 2008, October 27, 2009, and May 13,
809 2011 are associated with relatively dry, medium, and wet days, respectively) using the
810 TA model for (a) 0–0.2 and (b) 0–1.0 m.

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

812 estimation using the TA and SA models for (a) 0–0.2 and (b) 0–1.0 m for both cross
813 validation (CV) and external validation (EV). At 0–0.2 m, negative Nash-Sutcliffe
814 coefficient of efficiency values for three dates (October 22, 2008, August 27, 2009,
815 and October 27, 2009) are not shown. Spatial mean soil water content $S_{\hat{m}}$ on each
816 measurement day is also shown.

817 **Figure 9.** Difference between the Nash-Sutcliffe coefficient of efficiency (NSCE) of
818 soil water content estimation by both cross validation (CV) and external validation
819 (EV) using the TA and SA models as a function of space-invariant temporal anomaly
820 $A_{\hat{m}}$ for (a) 0–0.2 and (b) 0–1.0 m.

821 **Figure 10.** Difference between the Nash-Sutcliffe coefficient of efficiency (NSCE) of
822 soil water content evaluation by the cross validation using the TA and SA models as a
823 function of space-invariant temporal anomaly $A_{\hat{m}}$ for (a) 0–0.06 m of the Chinese
824 Loess Plateau hillslope and (b) 0–0.15 m of the GENCAI network in Italy.

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

	0–0.2 m		0–1.0 m	
	$M_{\hat{m}}$	EOF1	$M_{\hat{m}}$	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

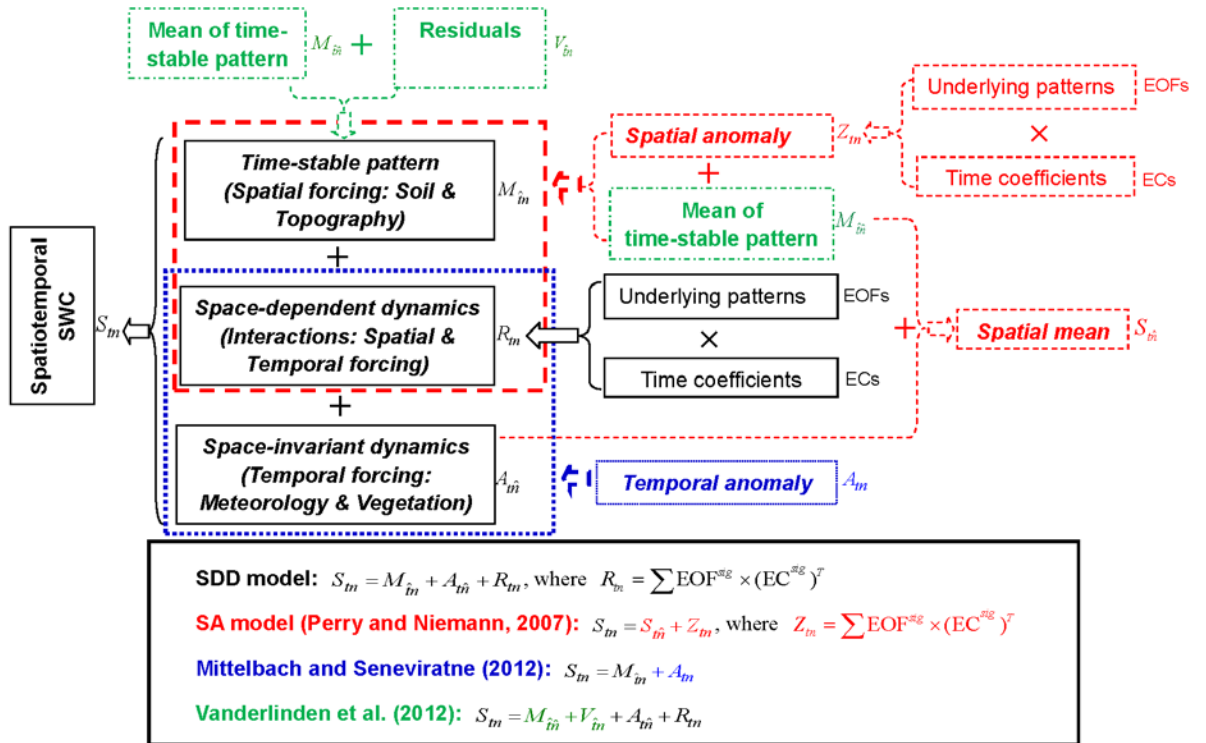


Fig. 1. Decomposition of spatiotemporal soil water content (SWC) in different models.

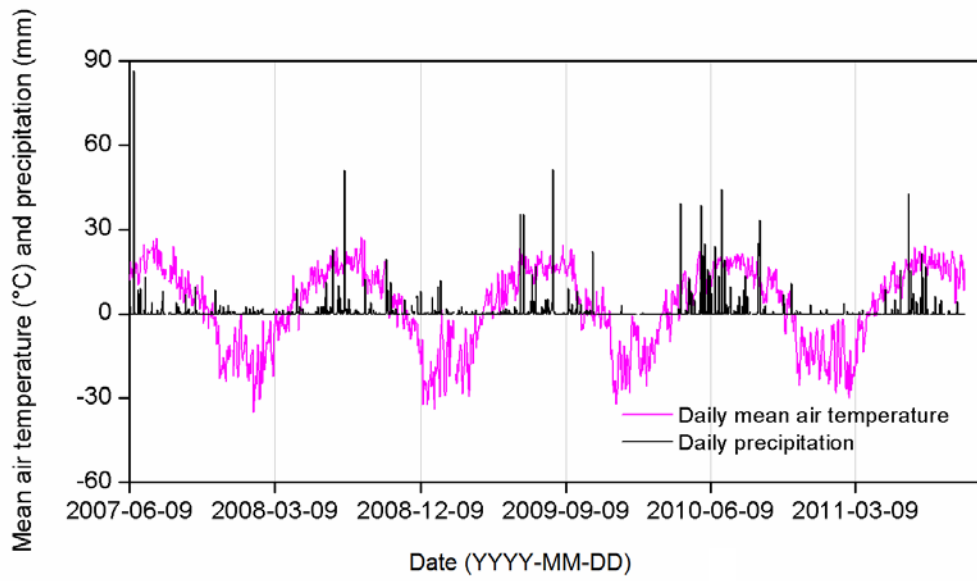


Fig. 2. Daily mean air temperature and precipitation during the study period.

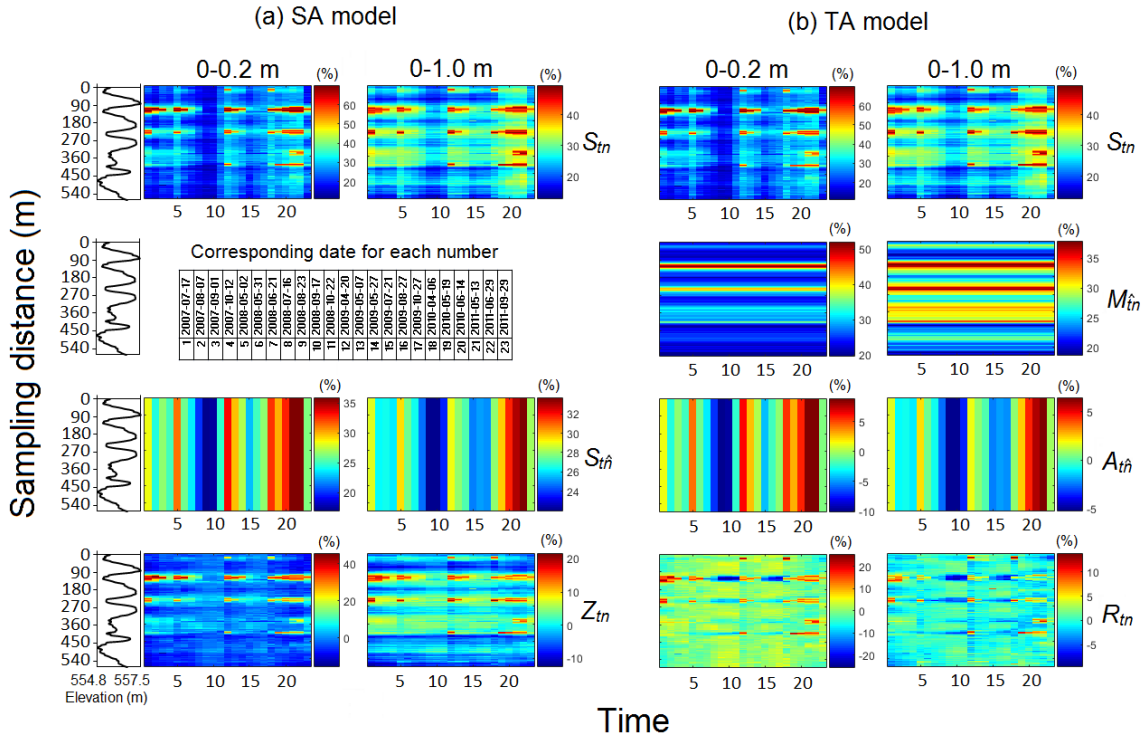


Fig. 3. Components of soil water content in (a) the SA model (spatial mean soil water content $S_{\hat{m}}$ and spatial anomaly Z_m) and in (b) the TA model (time-stable pattern $M_{\hat{m}}$, space-invariant temporal anomaly $A_{\hat{m}}$, and space-variant temporal anomaly R_m) for 0–0.2 and 0–1.0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

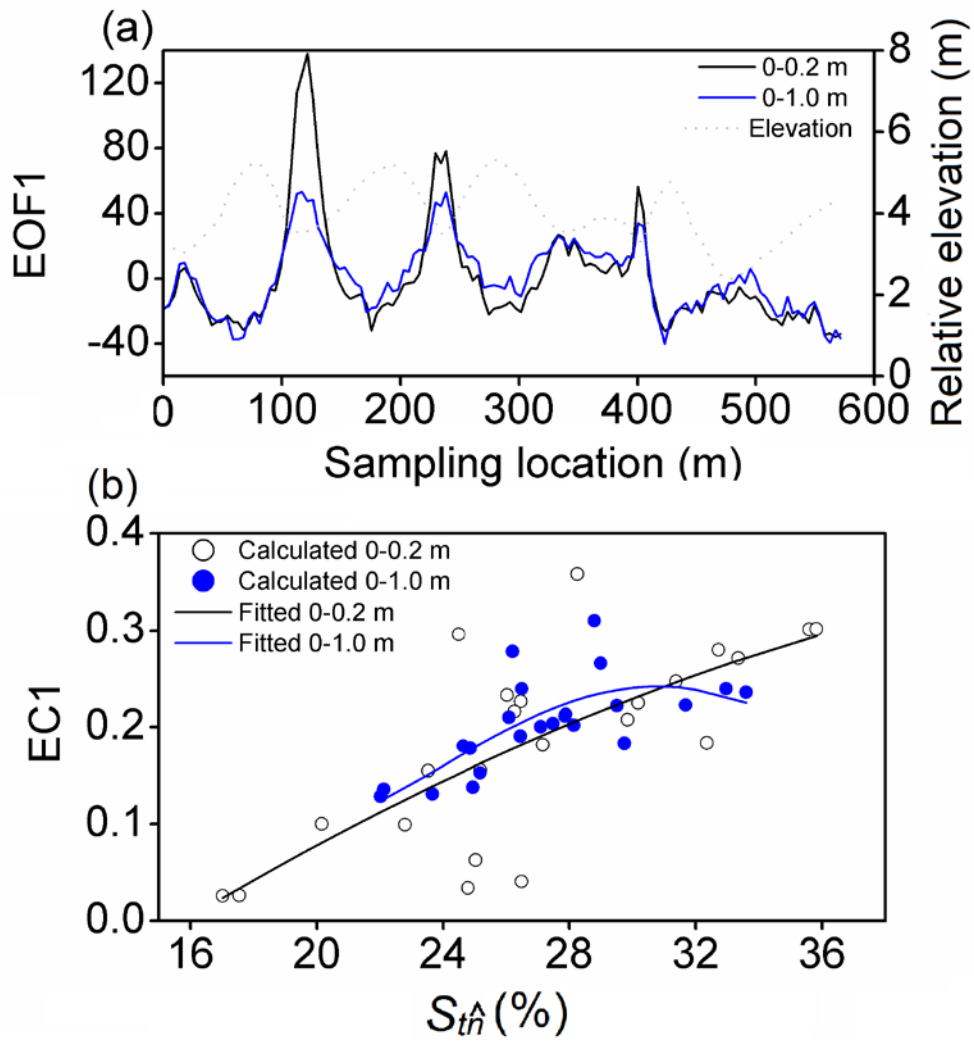


Fig. 4. (a) The EOF1 of the spatial anomaly Z_m and (b) relationships of associated EC1 versus spatial mean soil water content Z_m fitted by the cosine function (Eq. 4).

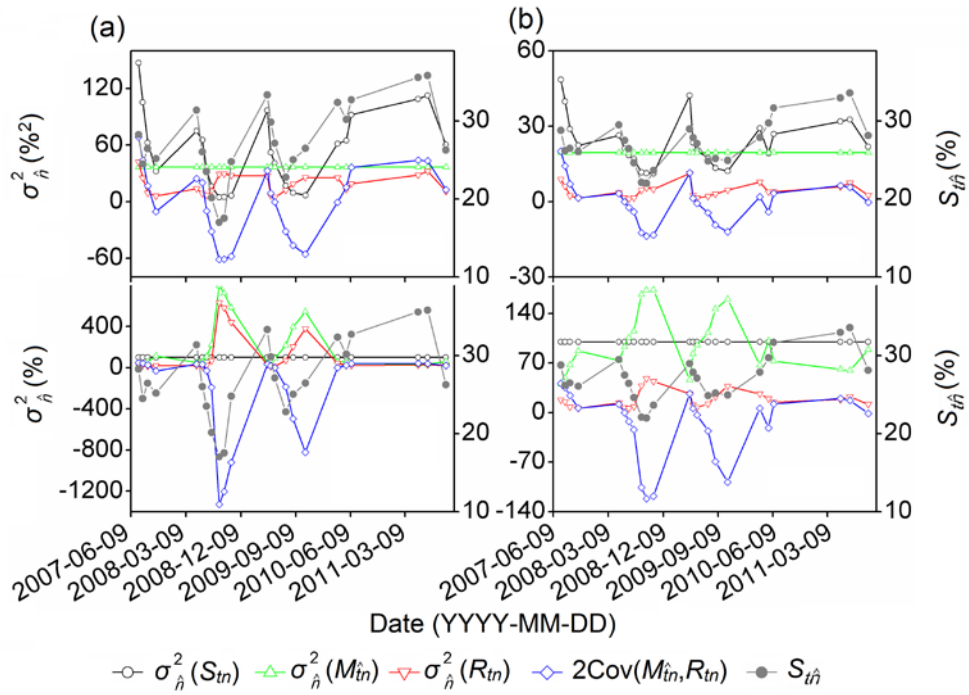


Fig. 5. Spatial variances of different components in Eq. (8) expressed in %² (upper panel) and as percentage (lower panel) for (a) 0–0.2 and (b) 0–1.0 m. Spatial mean soil water content S_{m} on each measurement day is also shown.

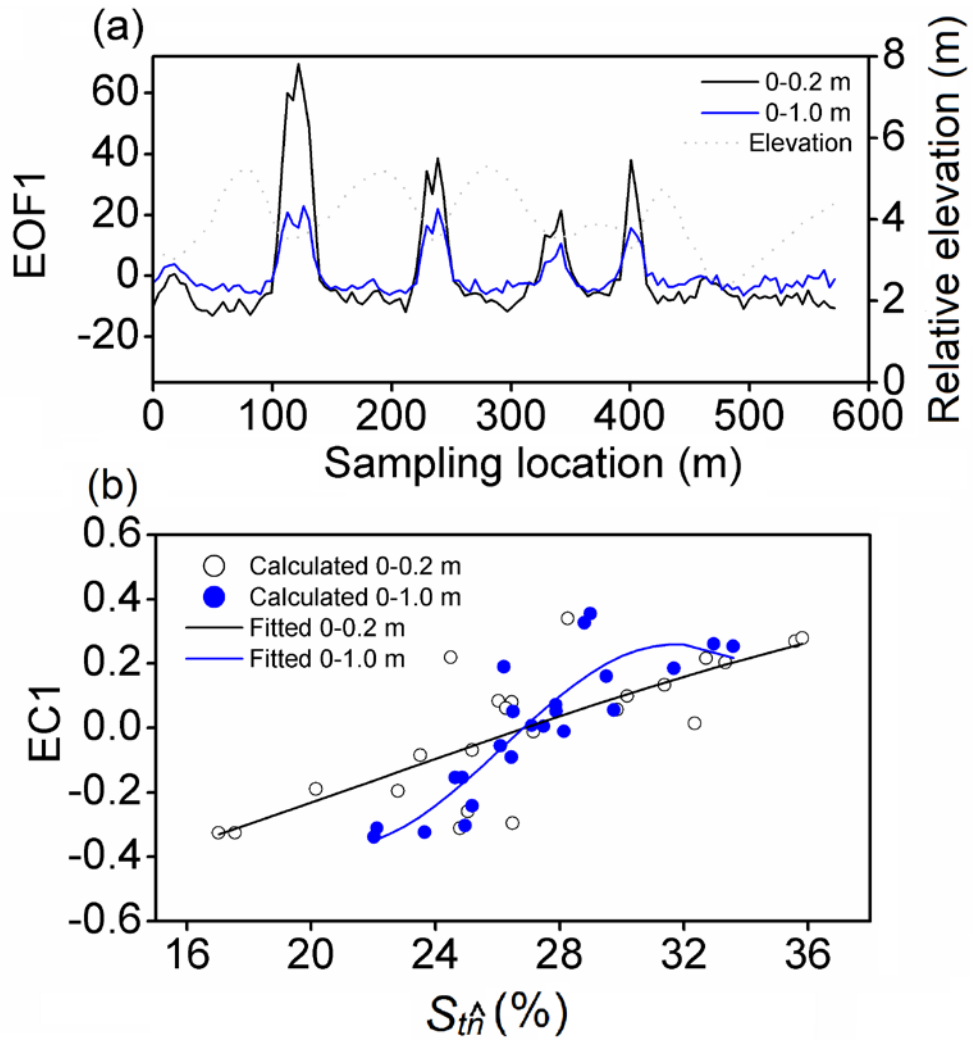


Fig. 6. (a) The EOF1 of the space-variant temporal anomaly R_{tn} and (b) relationships of associated EC1 versus spatial mean soil water content $S_{\hat{m}}$ fitted by the cosine function (Eq. 4).

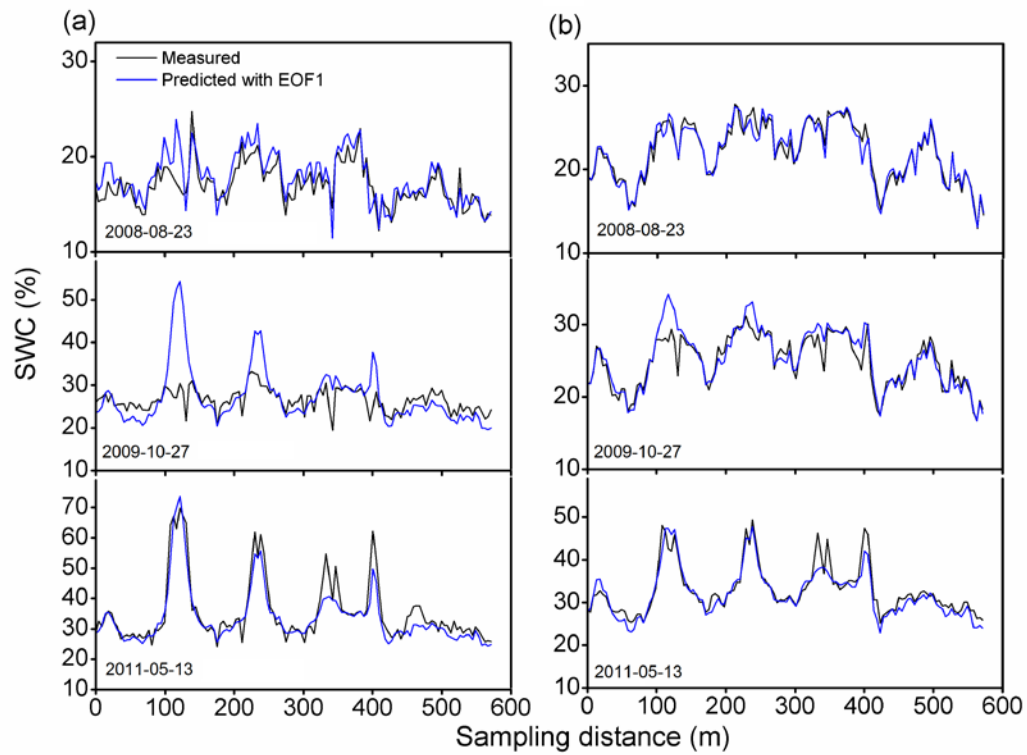


Fig. 7. Estimated soil water content (SWC) versus measured SWC for three dates at different soil water conditions (August 23, 2008, October 27, 2009, and May 13, 2011 are associated with relatively dry, medium, and wet days, respectively) using the TA model for (a) 0–0.2 and (b) 0–1.0 m.

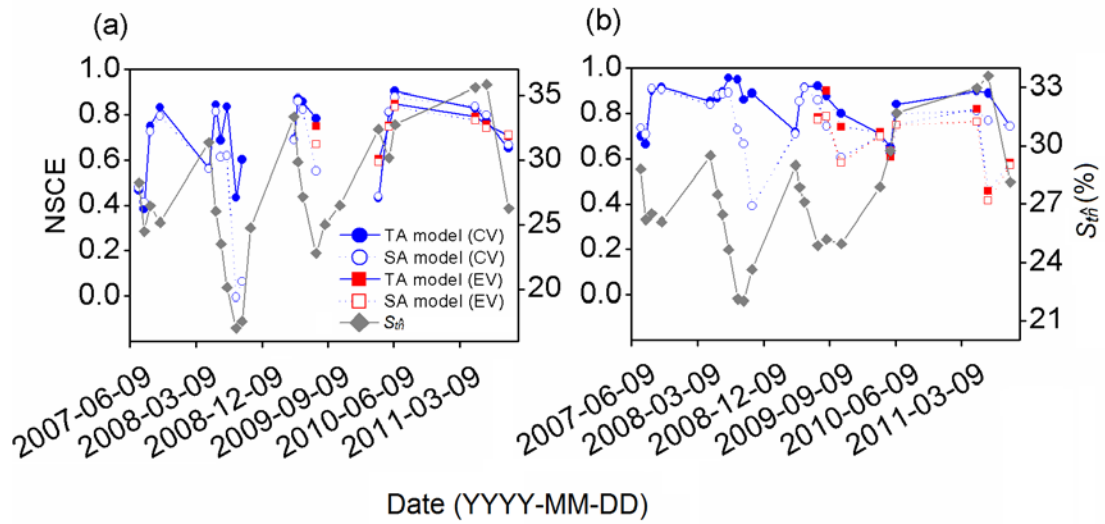


Fig. 8. The Nash-Sutcliffe coefficient of efficiency (NSCE) of soil water content estimation using the TA and SA models for (a) 0–0.2 and (b) 0–1.0 m for both cross validation (CV) and external validation (EV). At 0–0.2 m, negative Nash-Sutcliffe coefficient of efficiency values for three dates (October 22, 2008, August 27, 2009, and October 27, 2009) are not shown. Spatial mean soil water content S_m on each measurement day is also shown.

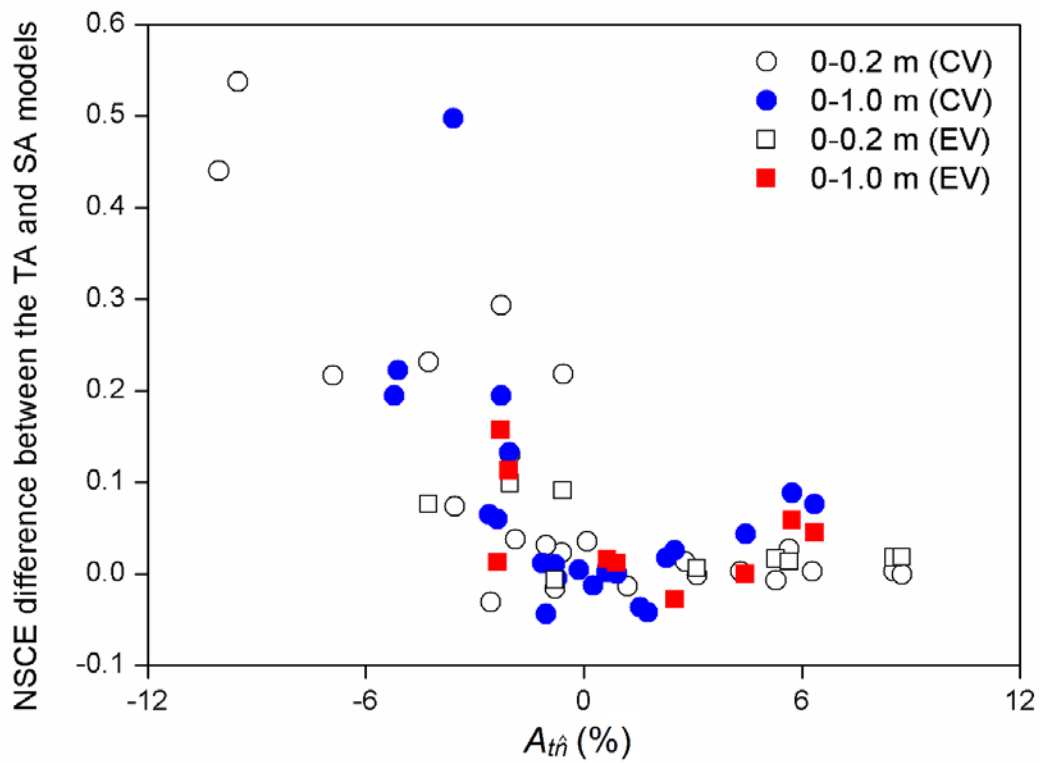


Fig. 9. Difference between the Nash-Sutcliffe coefficient of efficiency (NSCE) of soil water content estimation by both cross validation (CV) and external validation (EV) using the TA and SA models as a function of space-invariant temporal anomaly $A_{t\hat{h}}$ for (a) 0–0.2 and (b) 0–1.0 m.

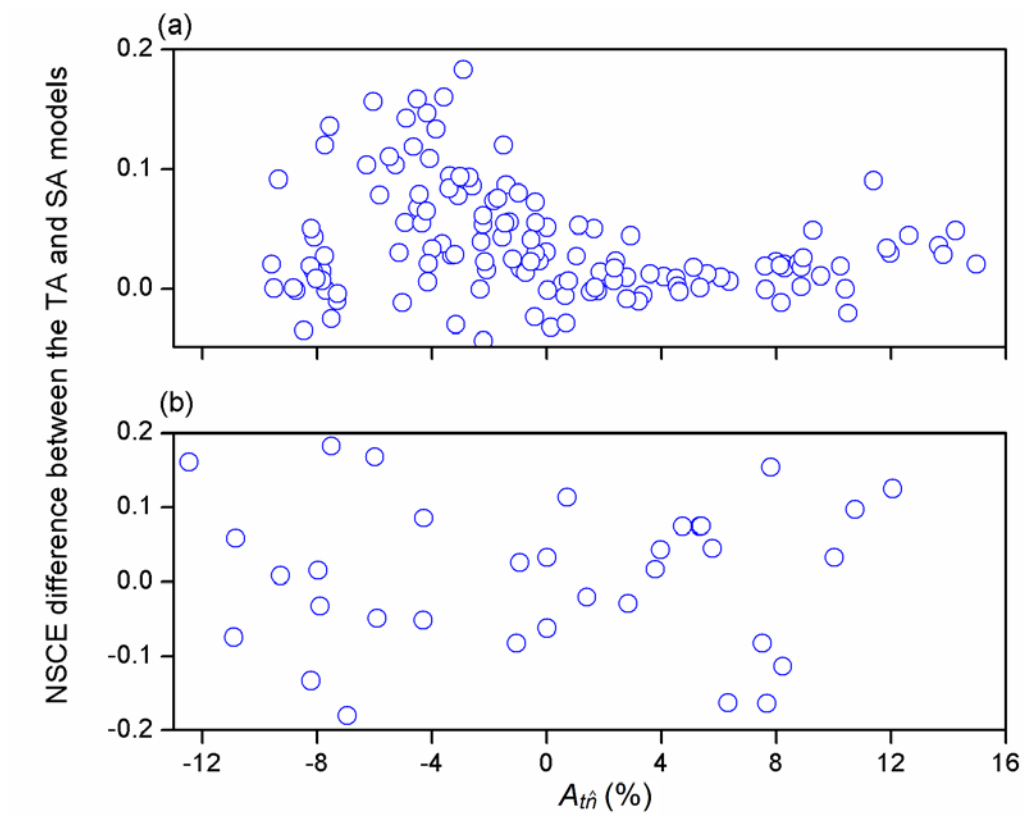


Fig. 10. Difference between the Nash-Sutcliffe coefficient of efficiency (NSCE) of soil water content evaluation by the cross validation using the TA and SA models as a function of space-invariant temporal anomaly A_{tn} for (a) 0–0.06 m of the Chinese Loess Plateau hillslope and (b) 0–0.15 m of the GENCAI network in Italy.