

Fuzzy clustering with spatial-temporal information

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Abstract

Clustering geographical units based on a set of quantitative features observed at several time occasions requires to deal with the complexity of both space and time information. In particular, one should consider (1) the spatial nature of the units to be clustered, (2) the characteristics of the space of multivariate time trajectories, and (3) the uncertainty related to the assignment of a geographical unit to a given cluster on the basis of the above complex features. This paper discusses a novel spatially constrained multivariate time series clustering for units characterised by different levels of spatial proximity. In particular, the Fuzzy Partitioning Around Medoids algorithm with Dynamic Time Warping dissimilarity measure and spatial penalization terms is applied to classify multivariate Spatial-Temporal series. The clustering method has been theoretically presented and discussed using both simulated and real data, highlighting its main features. In particular, the capability of embedding different levels of proximity among units, and the ability of considering time series with different length.

Keywords: Fuzzy Clustering, Partitioning Around Medoids, Time Series, Spatial information, Dynamic Time Warping, Tourism, Multilevel spatial proximity

1. Introduction

As Caiado et al. (2015) highlights, the (1) model- (2) feature- and (3) observation-based approaches are the main methodological veins developed in the past to aggregate units characterised by similar behaviour across time (for more details, see also Warren Liao, 2005; Caiado et al., 2015; D'Urso et al., 2016).

The idea behind the model-based clustering algorithms is to find the best mathematical/statistical model able to describe given time-varying data. The clustering is then performed on the parameter estimates (or on the residuals) of the fitted models (see, e.g., Piccolo, 1990; Maharaj, 1996; Garcia-Escudero & Gordaliza, 1999; Kalpakis et al., 2001; James & Sugar, 2003; Alonso & Maharaj, 2006; Caiado & Crato, 2010; Otranto, 2010; D'Urso et al., 2013b,a, 2016; D'Urso et al., 2017). Examples of model-based fuzzy clustering algorithms for univariate time series can be found in D'Urso et al. (2013a,b).

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23 Following the feature-based clustering approach, time series are clustered according to
24 one of their specific features, such as the autocorrelation function (ACF), the periodogram,
25 the density function or the wavelet information (see, e.g., Alonso & Maharaj, 2006; Caiado
26 et al., 2006, 2009; D’Urso & Maharaj, 2009; Maharaj & D’Urso, 2010, 2011; D’Urso &
27 Maharaj, 2012; D’Urso et al., 2014; Lafuente-Rego & Vilar, 2016; Vilar et al., 2017). In
28 the fuzzy clustering framework, both univariate and multivariate time series wavelet fea-
29 tures have been considered in Maharaj et al. (2010) and D’Urso & Maharaj (2012), while
30 frequency domains of univariate time series have been taken into account in Maharaj &
31 D’Urso (2011).

32 Observed time series, or suitable transformations, are instead the segmentation data
33 used in the observation-based approach (see, e.g., D’Urso, 2005a; Coppi et al., 2010, and
34 references therein). In the last decade, different fuzzy clustering algorithms have been
35 proposed for both univariate and multivariate time series (see, e.g., Coppi & D’Urso, 2002,
36 2003, 2006; D’Urso, 2005b; D’Urso et al., 2015, 2016; D’Urso et al., 2017; D’Urso et al.,
37 2017; Vilar et al., 2017).

38 Similarly, different methods have been suggested in the clustering literature to discover
39 spatial patterns for different kind of spatial units, e.g., urban areas or image pixels. The
40 main challenge these methods deal with is the identification of an appropriate algorithm
41 to capture both spatial dependence and spatial heterogeneity. Following the categorisation
42 suggested by Caiado et al. (2015), Fouedjio (2016) classifies clustering of spatial data
43 into four main approaches: (1) non-spatial clustering with geographical coordinates as
44 additional variables; (2) non-spatial clustering based on a spatial dissimilarity measure;
45 (3) spatially constrained clustering; (4) model-based clustering. An example of spatially
46 constrained fuzzy algorithm for urban areas is provided by Di Nola et al. (2000). Examples
47 of applications for image pixels segmentation can be found in Tolia & Panas (1998a,b);
48 Pham & Prince (1999); Liew et al. (2000, 2003); Pham (2001); Liew et al. (2003); Chuang
49 et al. (2006).

50 A fifth approach worth of notice consists in including a spatial penalty term in the
51 objective function of the clustering method, as suggested by Pham (2001). While this
52 proposal has been introduced for solving image segmentation problem, the idea beyond
53 can be easily extended to the clustering of geographical areas (Coppi et al., 2010).

54 When time information are available for space unit, the spatial time data array is a
55 three-way data array (i.e. arrays of the type: spatial objects \times variables \times occasions).
56 The spatial time data array \mathbf{X} can be reduced to a *bi*-dimensional array by combining two
57 of the three dimensions on the rows and assigning the remaining dimension to the columns
58 (Krishnapuram & Freg, 1992; Shekhar et al., 2015). This dimensionality reduction allows
59 for the classification of units by means of a traditional clustering technique at the expense
60 of information loss. To overcome this drawback, several clustering for spatial-temporal
61 series have been suggested in the literature. Following Disegna et al. (2017), clustering of
62 spatial-temporal series can be classified into: (i) non-spatial time series clustering based on
63 a spatial dissimilarity measure (Izakian et al., 2013); (ii) density-based clustering (Ester
64 et al., 1996; Wang et al., 2006; Birant & Kut, 2007; Ienco & Bordogna, 2016; Xie et al.,
65 2016); (iii) model-based clustering (Basford & McLachlan, 1985; Viroli, 2011; Torabi, 2014,

2016; Disegna et al., 2017); (iv) spatially constrained time series clustering (Hu & Sung, 2006; Coppi et al., 2010; Gao & Yu, 2016). Three-way data arrays have also been analysed by means of several fuzzy clustering algorithms (see, e.g., Sato & Sato, 1994; Sato et al., 1997; Gordon & Vichi, 2001; D’Urso, 2004, 2005a; Coppi et al., 2010). As for space data, Coppi et al. (2010) proposed the inclusion of the spatial penalty term in the objective function of a fuzzy clustering algorithm for spatial-temporal data too. The aim of this term is to reduce the membership degrees of all units contiguous to the generic i -th unit computed in all clusters but the c -th cluster to which the i -th unit belongs (Coppi et al., 2010).

In this study a generalisation of the fuzzy clustering algorithm with spatial penalization introduced by Coppi et al. (2010) is proposed. In particular, the innovation is threefold: firstly, we suggest to substitute the Euclidean distance with the Dynamic Time Warping (DTW) dissimilarity measure; secondly, we extend the Coppi et al. (2010)’s algorithm to the case in which data are characterised by different sources of spatial information; thirdly, a measure of spatial autocorrelation, the Fuzzy Moran (FM)’s index, is defined to study the autocorrelation of the final imprecise partition when several spatial penalty terms are considered.

The DTW dissimilarity measure has been selected instead of other more traditional distance measures, such as the well known Euclidean distance, mainly for its flexibility, the possibility to simultaneously consider both intensity and dynamic existing between time series, and thanks to its ability to compute distance among multivariate time series not necessarily of the same length.

The necessity to consider more than one spatial penalty term in the clustering algorithm is motivated by practical case studies in which units are characterised by different levels, or concepts, of proximity. For instance, European region are classified into three levels of Nomenclature of Territorial Units for Statistics (NUTS) geography classification and any clustering analysis of European cities should take into consideration these three levels.

Therefore, the Dynamic Time Warping Fuzzy C -Medoids for Spatial-Temporal Trajectories (DTW-FCMd-STT) clustering algorithm with penalty terms is proposed and described in this manuscript.

The paper is structured as follows: in section 2 the suggested algorithm is described and discussed in depth; in section 3 different simulated case studies are presented in order to show the main features of the algorithm; in section 4 the methodology is illustrated by analysing real data describing the behaviour of the tourism flows in a destination, i.e. spatial region. section 5 concludes.

2. The methodology

The starting point is represented by a spatial time data array (three-way data array), algebraically formalised as (D’Urso, 2000, 2004, 2005a):

$$\mathbf{X} \equiv \{x_{ijt} : i = 1, \dots, I; j = 1, \dots, J; t = 1, \dots, T\} \quad (1)$$

104 where i indicates the generic unit (geographical area or region), j the variable, and t the
 105 generic time; x_{ijt} is the value of the j -th variable observed for the i -th unit at time t .

Notice that the time data array \mathbf{X} can be synthetically represented by means of a *bi*-dimensional matrix combining two of the three indices i, j, t on the rows and assigning the remaining index to the columns. For instance, the time data array can be defined as the set of *bi*-dimensional matrices $\mathbf{X}_i, \mathbf{X}_t$, or \mathbf{X}_j as follows:

$$\begin{aligned}\mathbf{X}_i &\equiv \{x_{ijt} : j = 1, \dots, J; t = 1, \dots, T\} \\ \mathbf{X}_t &\equiv \{x_{ijt} : i = 1, \dots, I; j = 1, \dots, J\} \\ \mathbf{X}_j &\equiv \{x_{ijt} : i = 1, \dots, I; t = 1, \dots, T\}.\end{aligned}$$

106 We also assume to have K additional pieces of information on spatial location of each
 107 units in relation with the others, i.e., K different levels of spatial proximity. Each level of
 108 proximity is defined by a $(I \times I)$ symmetric data matrix \mathbf{P}_k ($k = 1, \dots, K$), whose generic
 109 entry $p_{kii'}$ is a measure of a particular definition of spatial proximity between the i -th and
 110 i' -th units ($i, i' = 1, \dots, I$), where $0 \leq p_{kii'} \leq 1$ and $p_{kii} = 0$. For instance, $p_{kii'} = 1$ if
 111 the two areas are contiguous, $p_{kii'} = 0$ otherwise. Alternatively, $p_{kii'}$ could be inversely
 112 proportional to the geographic distance between i and i' . We will further illustrate different
 113 kind of proximity matrix in section 2.2.

114 Figure 1 graphically represents the bundle of available information and the dimensions
 115 of the data array typically used in spatial-temporal analysis.

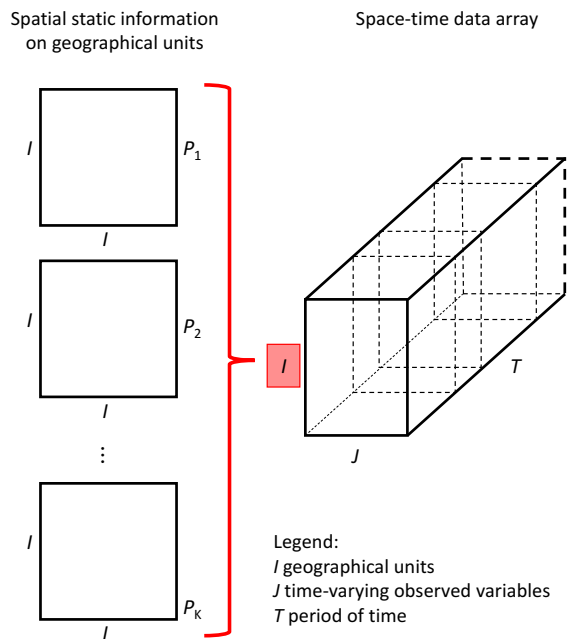


Figure 1: Spatial-temporal data array

116 For classification purpose, the i -th multivariate time trajectory is formalized by the

117 matrix $\mathbf{X}_i \equiv \{\mathbf{x}_{it} : t = 1, \dots, T\}$, where $\mathbf{x}_{it} \equiv (x_{i1t}, \dots, x_{ijt}, \dots, x_{iJt})$, $i = 1, \dots, I$, $t =$
 118 $1, \dots, T$.

119 2.1. Dynamic Time Warping

120 The Dynamic Time Warping (DTW) (Velichko et al., 1970; Berndt, 1994; Izakian et al.,
 121 2015; D’Urso et al., 2018) allows to locally stretch or compress multivariate time series to
 122 make their shape as similar as possible.

123 To this end, the functions that allow to remap each multivariate time series need to be
 124 identified. This kind of function is called warping function and its aim is to “realign” the
 125 time indices of the multivariate time series.

126 Given a “query” (or test) multivariate time series \mathbf{X}_i and a “reference” multivariate
 127 time series, $\mathbf{X}_{i'}$, with length T and T' ($T \geq T'$) respectively, the total distance between \mathbf{X}_i
 128 and $\mathbf{X}_{i'}$ is computed by means of the warping path. The warping path allows to compare
 129 each data point in \mathbf{X}_i with the closest data point in $\mathbf{X}_{i'}$, and is defined as

$$\Phi_l = (\varphi_l, \psi_l), \quad l = 1, \dots, L.$$

130 under the following constraints.

- 131 1. boundary condition: $\Phi_1 = (1, 1)$, $\Phi_L = (T, T')$;
- 132 2. monotonicity condition: $\varphi_1 \leq \dots \leq \varphi_l \leq \dots \leq \varphi_L$ and $\psi_1 \leq \dots \leq \psi_l \leq \dots \leq \psi_L$.

133 The total dissimilarity between the two “warped” multivariate time series is:

$$\sum_{l=1}^L d(\mathbf{x}_{i, \varphi_l}, \mathbf{x}_{i', \psi_l}) m_{l, \Phi}$$

134 where $m_{l, \Phi}$ is a local weighting coefficient, and $d(., .)$ is, usually, the Euclidean distance
 135 for multivariate time series (Giorgino et al., 2009). Since there are several warping curves,
 136 the DTW dissimilarity measure is the one which correspond to the optimal warping curve,
 137 $\hat{\Phi}_l = (\hat{\varphi}_l, \hat{\psi}_l)$, ($l = 1, \dots, L$), which minimizes the total dissimilarity between \mathbf{X}_i and $\mathbf{X}_{i'}$:

$$D(\mathbf{X}_i, \mathbf{X}_{i'}) = \min_{\Phi_l} \sum_{l=1}^L d(\mathbf{x}_{i, \varphi_l}, \mathbf{x}_{i', \psi_l}) m_{l, \Phi} = \sum_{l=1}^L d(\mathbf{x}_{i, \hat{\varphi}_l}, \mathbf{x}_{i', \hat{\psi}_l}) m_{l, \hat{\Phi}}. \quad (2)$$

138 The DTW dissimilarity measure is particularly useful when comparing multivariate
 139 time series. First, by preserving the time ordering of the sequence, the DTW goes beyond
 140 the instantaneous features of time data. Indeed, DTW dissimilarity measure copes with
 141 both the instantaneous and the variational features of the multivariate time trajectories,
 142 i.e., the instantaneous position of the trajectories and their dynamic evolution over time,
 143 thus providing a more complete comparison that takes into account also the different rates
 144 at which phenomena change over times. Second the DTW dissimilarity measure is also
 145 more flexible than the Euclidean distance since it allows for comparison of multivariate time
 146 series of different lengths. Third, no assumptions are required regarding the multivariate

147 time series properties. Furthermore, Euclidean distance is calculated in a one-to-one man-
 148 ner, while DTW dissimilarity measure tries to find the best warping. Finally, by taking
 149 explicitly into account the ordering of the observations, DTW also deals with the presence
 150 of possible time shifts in the data.

151 For all these reasons, DTW is now usually adopted as a suitable alternative to Euclidean
 152 distance in time series cluster analysis (see, among others, Berndt, 1994; Oates et al., 1999;
 153 Jeong et al., 2011; Petitjean et al., 2011; Begum et al., 2015; Izakian et al., 2015; Mure et al.,
 154 2016) In particular, Ding et al. (2008) and Rakthanmanon et al. (2012) experimentally
 155 proved the effectiveness of DTW in data mining problems—like time series clustering is—
 156 with respect to other distance measures.

157 Furthermore, while DTW is more computationally demanding than Euclidean distance,
 158 by adopting a Partitioning-Around-Medoids (PAM, Kaufman & Rousseeuw, 2005) ap-
 159 proach (see section 2.3 below), the distance matrix should be computed only once at the
 160 start of the overall clustering procedure (D’Urso et al., 2018).

161 2.2. Dealing with space: proximity matrix

162 When dealing with spatial data the within group dispersion has to be minimised and the
 163 spatial autocorrelation between contiguous spatial units has to be taken into consideration.
 164 This spatial information can be analytically embedded in the clustering process using a
 165 “proximity” matrix, say \mathbf{P} , that is a symmetric matrix of order I whose elements signal the
 166 proximity between two spatial areas (Pham, 2001; Coppi et al., 2010). In the literature,
 167 there are different ways of defining proximity and consequently there are different ways of
 168 constructing proximity matrices among spatial units (Gordon, 1999; Páez & Scott, 2005).
 169 Two of the most common definitions are based on connectivity, i.e. travel time or distance
 170 between pairs of units, and physical contiguity.

171 Connectivity can be coped with by means of a proximity matrix \mathbf{P} whose elements
 172 are given by the inverse of a generic measure of the distance between i and i' (distance
 173 between the two spatial units, trip duration and/or cost, etc.), normalized to range in
 174 $[0, 1]$. The more two spatial areas are connected, the lower is the value in the proximity
 175 matrix. Obviously, diagonal elements are all equal to 0.

176 Spatial contiguity, on its turn, can be specified in several ways. For instance, two
 177 spatial units can be contiguous either if they are adjacent (neighbours) or if they belong
 178 to the same macro-area, even if they are not adjacent. In this case, \mathbf{P} is constructed as a
 179 symmetric matrix with 0 diagonal elements and with off-diagonal elements given by:

$$180 \quad p_{ii'} = \begin{cases} 1 & \text{if } i \text{ is contiguous to } i' \\ 0 & \text{otherwise} \end{cases} \quad i = 1, \dots, I, i \neq i'. \quad (3)$$

180 2.3. The DTW-Fuzzy C-Medoids clustering algorithm for Spatial-Temporal Trajectories 181 (DTW-FCMd-STT)

182 In this paper, following a PAM approach in a fuzzy framework, the Fuzzy C -Medoids
 183 (FCMd, Krishnapuram et al., 2001) clustering algorithm is adopted. With respect to stan-
 184 dard (crisp) clustering algorithms, fuzzy clustering algorithms are generally more efficient—
 185 dramatic changes in the value of cluster membership are less likely to occur in estimation

186 procedures—and they are less affected by both local optima and convergence problems
 187 (Everitt et al., 2001; Hwang et al., 2007). With complex data as multivariate time series
 188 are, it could be difficult to identify a clear boundary between clusters in real applications.
 189 In this sense, fuzzy clustering appears more attractive than the crisp clustering methods
 190 ?Wedel & Kamakura (2000). Finally, the membership degrees produced by fuzzy cluster-
 191 ing methods, that indicate the belonging of each unit to each cluster, also indicate whether
 192 there is a second-best cluster almost as good as the best cluster, a scenario which crisp
 193 clustering methods cannot uncover Everitt et al. (2001).

194 Regarding the choice of the fuzzy clustering method, with respect to Fuzzy C -Means
 195 (FCM, Bezdek, 1981), FCMd allows for more appealing and easy to interpret results of the
 196 final partition (Kaufman & Rousseeuw, 2005) by obtaining non-fictitious representative
 197 time series (i.e. the medoids) as final result (see section 2.6).

198 Dealing with Spatial-Temporal trajectories, possible spillover effects between adjacent
 199 units have to be taken into account. As observed in section 2.2, since there could be
 200 different, say K ($K \geq 1$), definitions of proximity, K spatial penalty terms are added to
 201 the objective function. Following Pham & Prince (1999) and Coppi et al. (2010), the
 202 DTW-Fuzzy C -Medoids clustering algorithm for Spatial-Temporal Trajectories (DTW-
 203 FCMd-STT) is then formalised as follows:

$$\left\{ \begin{array}{l} \min : \sum_{i=1}^I \sum_{c=1}^C u_{ic}^m D(\mathbf{X}_i, \tilde{\mathbf{X}}_c) + \sum_{k=1}^K \frac{\beta_k}{2} \sum_{i=1}^I \sum_{c=1}^C u_{ic}^m \sum_{i'=1}^I \sum_{c' \in C_c} p_{kii'} u_{i'c'}^m \\ s.t. \quad \sum_{c=1}^C u_{ic} = 1, u_{ic} \geq 0 \end{array} \right. \quad (4)$$

204 where \mathbf{X}_i and $\tilde{\mathbf{X}}_c$ are the multivariate time trajectories of the i -th spatial unit and of the
 205 c -th spatial medoid ($c = 1, \dots, C$), respectively; $D(\cdot, \cdot)$ is the DTW dissimilarity measure
 206 for multivariate spatial time series; $m > 1$ is the fuzziness parameter; $\beta_k \geq 0$ is the
 207 tuning parameter of the k -th spatial information; $p_{kii'}$ is the generic element of the $(I \times I)$
 208 “proximity” matrix \mathbf{P}_k ; C_c is the set of the C clusters, with the exclusion of cluster c ; u_{ic}
 209 is the membership degree of the unit i to the cluster c .

210 The objective function in (4) is made up by two distinguished terms:

- 211 • the time dependent term (see section 2.3.1)

$$\sum_{i=1}^I \sum_{c=1}^C u_{ic}^m D(\mathbf{X}_i, \tilde{\mathbf{X}}_c); \quad (5)$$

- 212 • the spatial dependent term

$$\sum_{k=1}^K \frac{\beta_k}{2} \sum_{i=1}^I \sum_{c=1}^C u_{ic}^m \sum_{i'=1}^I \sum_{c' \in C_c} p_{kii'} u_{i'c'}^m \quad (6)$$

213 which is the sum of K spatial penalty terms (see section 2.3.2).

214 The two terms (5) and (6) are computed over the same data range, i.e., over the same
 215 observations. In the clustering process, one term could dominate the other depending on
 216 the data at hand. The way in which both terms contribute to the clustering results will
 217 be clarified in sections 2.3.1-2.3.2.

218 The optimal iterative solution for the objective function in (4) is:

$$u_{ic} = \frac{\left[D(\mathbf{X}_i, \tilde{\mathbf{X}}_c) + \sum_{k=1}^K \beta_k \sum_{i'=1}^I \sum_{c' \in C_c} p_{kii'} u_{i'c'}^m \right]^{-\frac{1}{m-1}}}{\sum_{c'=1}^C \left[D(\mathbf{X}_i, \tilde{\mathbf{X}}_{c'}) + \sum_{k=1}^K \beta_k \sum_{i'=1}^I \sum_{c'' \in C_{c'}} p_{kii'} u_{i'c''}^m \right]^{-\frac{1}{m-1}}} \quad (7)$$

219 As a final remark, the overall optimization of the objective function in (4) ensures that
 220 the cohesion within clusters is maximized and that the spatial autocorrelation existing in
 221 the data at hand is properly coped with, simultaneously, as it will be explained in the
 222 following.

223 2.3.1. Time dependent term

224 The time dependent term (5) is the within cluster dispersion due to the time-varying
 225 features of multivariate trajectories. As observed in section 2.1, in this term the whole time
 226 information is inherited by the Dynamic Time Warping measure, that takes into account
 227 both the instantaneous and the variational features of the multivariate time trajectories.
 228 When there are no spatial information, the time dependent term (5) coincides with the
 229 Dynamic Time Warping Fuzzy C -Medoids (DTW-FCMd) for multivariate time trajectories
 230 introduced by D'Urso et al. (2018).

231 2.3.2. Spatial dependent term

232 The spatial dependent term (6) suitably allows the objective function to incorporate
 233 different sources of spatial information. The term (6) is the sum of K ($K \geq 1$) spatial
 234 penalty terms (Pham, 2001; Coppi et al., 2010), one for each definition of proximity among
 235 areas considered. In this way, the clustering method captures the information connected
 236 to the different levels of proximity (multilevel proximity). For instance, we can consider
 237 the simple case illustrated in Figure 2 in which 5 units, i.e. towns, and 2 macroarea, i.e.
 238 valleys, are considered. In this specific case, two kinds of proximity can be defined: (i)
 239 proximity among towns (level 1 proximity); belonging to the same valley (level 2 proximity).
 240 Therefore, four different scenarios can be identified: 1) two towns (a_1 and a_2) are close to
 241 each other (level 1 proximity) and they belong to the same valley (level 2 proximity); 2)
 242 two towns (a_1 and b_1) are close to each other (level 1 proximity) but they do not belong
 243 to the same valley; 3) two towns (a_1 and a_3) are not close to each other but they belong
 244 to the same valley (level 2 proximity); 4) two towns (a_1 and b_2) are not close to each other
 245 and they do not belong to the same valley.

246 In each spatial penalty term two parameters are relevant, the proximity matrix \mathbf{P}_k , and
 247 the tuning parameter β_k .

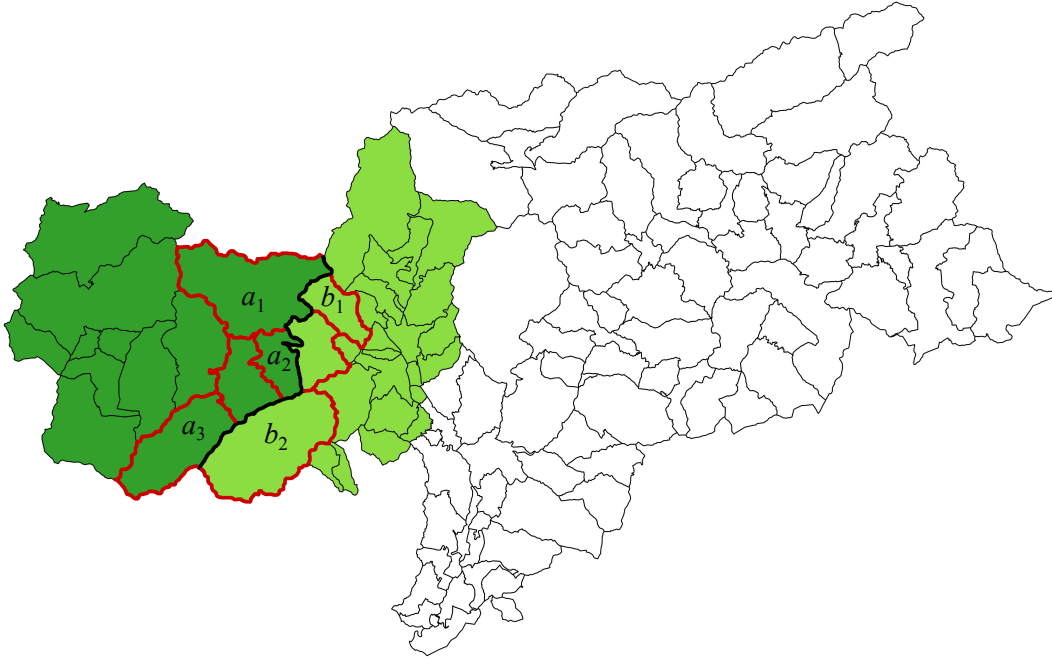


Figure 2: Example of proximity among areas where a_1 , a_2 , a_3 , b_1 , and b_2 are towns and the light green and dark green areas represent two valleys

248 The role of the k -th proximity matrix, \mathbf{P}_k , is to increase the membership degree of unit
 249 i in cluster c and, at the same time, to increase the membership degrees of the units that
 250 are connected, in some way, to i in cluster c , while reducing these membership degrees
 251 in the other clusters. We define this spatial smoothing as “proximity effect”, where, as
 252 previously observed, the concept of proximity is vast enough to encompass different types of
 253 connectivity between areas. The tuning parameter β_k must be set depending on the spatial
 254 autocorrelation among data (see section 2.5 below). β_k could enhance the proximity effect
 255 due to \mathbf{P}_k if the spatial autocorrelation between units is high, e.g., if the features of a spatial
 256 unit display a certain degree of concordance with those of its neighbours. Otherwise, β_k
 257 could counterbalance, if not neutralise at all, the proximity effect, if there is relatively low
 258 spatial autocorrelation between areas. Then, the greater the value of β_k , the greater is the
 259 weight of the concept of proximity ascribed to it in the clustering process. Let say that
 260 β_1 corresponds to the distance between areas, and β_2 to the belonging to the same macro-
 261 area, then, if $\beta_1 > \beta_2$, “closeness” plays a major role than “belonging” in the optimization
 262 process.

263 As already observed, the choice of the value of β_k is data dependent. Coppi et al.
 264 (2010) observed that the choice should be made according to a measure of a within cluster
 265 spatial autocorrelation (see section 2.5), to avoid that the spatial smoothing induced by
 266 the proximity matrix overcome the cluster separation. Indeed, an excessively high value
 267 of one or more β_k ’s could constraint all neighbour units to be classified in one cluster,
 268 regardless the features observed. A heuristic procedure for a custom-made choice of β_k ’s

269 is illustrated in section 4.

270 Finally, it should be stressed that by combining \mathbf{P}_k and β_k in the clustering process,
271 we are able to take into account also the spatial autocorrelation which is more informative
272 than the spatial proximity alone.

273 2.3.3. *A remark on the use of spatial information*

274 As highlighted in the Introduction, in spatial clustering there are different approaches
275 to incorporate spatial information in a clustering framework. In particular, spatial infor-
276 mation can be represented in a clustering method by considering the contiguity/adjacencies
277 between each pair of territorial (spatial) units (Gordon, 1999). This information is usu-
278 ally formalized in the clustering method by means of contiguity/adjacencies constraints
279 or suitable spatial weights associated to distance measures. This approach is preferred in
280 hierarchical clustering (i.e. agglomerative) or in relational clustering where the distance
281 measure is taken for each pair of territorial units. In doing so the spatial information is
282 represented algebraically by a squared matrix (called either contiguity matrix or spatial
283 matrix) associated to the squared distance matrix. Each element of this matrix represents
284 the territorial proximity between two units that can be represented by either dichotomous
285 values (0 or 1), indicating if the units are neighbouring or not, or quantitative values
286 representing the road distances or travel times.

287 In the literature, another well-known approach used to incorporate spatial information
288 in the clustering procedure is to introduce a suitable penalty term in the objective function
289 used in the optimization procedure for clustering territorial units (see, e.g., Pham, 2001; ?;
290 Coppi et al., 2010). This approach is used in non-hierarchical framework (e.g. hard or fuzzy
291 C -means clustering and hard or fuzzy partitioning around medoids procedures, as the hard
292 or fuzzy C -medoids clustering), where the spatial information cannot be represented by
293 squared matrix. In fact, in these cases, the dimension of the distance matrix is rectangular
294 (the matrix contains values representing, e.g., the distance between each territorial unit
295 and each centroid or between each territorial unit and each medoid, where centroids and
296 medoids are the prototypes representing the clusters). This approach is quite common in
297 the spatial clustering literature. As remarked by Pham (2001), “a classical approach to
298 incorporating spatial information is to penalize the [...] objective function [of the fuzzy
299 clustering] to constrain the behavior of the membership functions, similar to methods used
300 in regularization and Markov random field (MRF) theory (?). This penalty can be used
301 to discourage unlikely or undesirable configurations in the membership functions, such as
302 a high membership value immediately surrounded by low values of the same class”. The
303 Markov random field (MRF) theory has been used by ? “which used standard first order
304 differences as a penalty to force membership values to be similar to neighbouring values.
305 The main problem with such a penalty function, however, is that it can drastically alter
306 the characteristics of the membership function in an undesirable fashion. For example, first
307 order differences will cause membership functions to be nearly piecewise constant. Second
308 order differences will cause membership functions to be more smooth. However, depending
309 on the value of the $[m]$ parameter, this may contradict the desired characteristics of the
310 membership functions. [In our method], the objective function [see formula (4)] includes a

311 penalty term that is reminiscent of MRF priors but is consistent with the desired behavior
 312 of the membership functions dictated by the value of the m parameter” (Pham, 2001). As
 313 remarked before, the use of penalty terms for taking into account the spatial proximity is
 314 largely used in the literature, in different research areas (see, among others, ?????????).
 315 Then, it is a consolidated methodological approach in the spatial clustering analysis.

316 Notice that, since our clustering method classify territorial units following a non-
 317 hierarchical approach, we cannot consider the spatial information represented by conti-
 318 guity or spatial measures (that compare pair of units) formalized as constraints or weights
 319 associated to distance matrix (as in the hierarchical approach). In addition, since we con-
 320 sider different levels of contiguity, considering different adjacency matrices as weights to
 321 embed would considerably increase the complexity of the procedure. Nonetheless, as will
 322 be remarked in the Conclusions, in the future we will explore the possibility to take into
 323 account the spatial information in the clustering process following another clustering ap-
 324 proach, i.e. the fuzzy relational method (Kaufman & Rousseeuw, 2005; D’Urso, 2015).
 325 We will also investigate the computational and operational complexity of this alternative
 326 clustering procedure (scalability, etc.).

327 2.4. Validity measure

328 In general, internal validity measures provide useful guidelines in the identification of
 329 the best partition (Handl et al., 2005; D’Urso, 2015). Suitable measures for fuzzy clustering
 330 algorithm have been suggested by Xie & Beni (1991) and Campello & Hruschka (2006).

331 The Xie and Beni cluster validity index (Xie & Beni, 1991) is the ratio between com-
 332 pactness and separation among clusters and it can be expressed as:

$$XB = \frac{\sum_{i=1}^I \sum_{c=1}^C u_{ic}^p D(\mathbf{X}_i, \tilde{\mathbf{X}}_c)}{I \min_{p \neq q} D(\tilde{\mathbf{X}}_p, \tilde{\mathbf{X}}_q)} \quad (8)$$

333 where $(p, q) \in \{1, \dots, C\}$. The smaller XB , the more compact and separate are the
 334 clusters.

335 The Fuzzy Silhouette (FS) index (Campello & Hruschka, 2006) is computed as the
 336 weighted average of individual silhouettes width, λ_i , (Kaufman & Rousseeuw, 2005), with
 337 weights derived from the fuzzy membership matrix $\mathbf{U} = \{u_{ic} : i = 1, \dots, I; c = 1, \dots, C\}$
 338 as follows:

$$FS = \frac{\sum_{i=1}^I (u_{ip} - u_{iq})^\alpha \cdot \lambda_i}{\sum_{i=1}^I (u_{ip} - u_{iq})^\alpha}, \quad \lambda_i = \frac{(b_i - a_i)}{\max\{b_i, a_i\}} \quad (9)$$

339 Here, a_i is the average distance between the i -th unit and the units belonging to the
 340 cluster p ($p = 1, \dots, C$) with which i is associated with the highest membership degree; b_i
 341 is the minimum (over clusters) average distance of the i -th unit to all units belonging to the
 342 cluster q with $q \neq p$; $(u_{ip} - u_{iq})^\alpha$ is the weight of each λ_i calculated upon \mathbf{U} , where p and q
 343 are, respectively, the first and second best clusters (accordingly to the membership degree)

344 to which the i -th unit is associated; $\alpha \geq 0$ is an optional user defined weighting coefficient.
 345 The traditional (crisp) Silhouette coefficients is obtained by setting $\alpha = 0$. The higher
 346 the value of FS , the better the assignment of the units to the clusters simultaneously
 347 obtaining the minimisation of the intra-cluster distance and the maximisation of the inter-
 348 cluster distance.

349 2.5. Spatial autocorrelation

350 In this paper, we introduce a new measure of spatial autocorrelation to assess the
 351 post-cluster autocorrelation between units, the Fuzzy Moran (FM) index. This index is a
 352 multivariate fuzzy generalisation of the Moran’s index (Gittleman & Kot, 1990) and it is
 353 a generalization of the spatial autocorrelation measure introduced by Coppi et al. (2010).
 354 The idea of the FM index is to compute the spatial autocorrelation between classified
 355 units in which both the fuzzy membership matrix \mathbf{U} and the spatial proximity matrices
 356 \mathbf{P}_k are considered. The FM index is defined as follows:

$$FM = \frac{tr \left[\bar{\mathbf{X}}' \mathbf{U}_c^{\frac{1}{2}} \tilde{\mathbf{P}} \mathbf{U}_c^{\frac{1}{2}} \bar{\mathbf{X}} \right]}{tr \left[\bar{\mathbf{X}}' \mathbf{U}_c^{\frac{1}{2}} \text{diag}(\tilde{\mathbf{P}}) \mathbf{U}_c^{\frac{1}{2}} \bar{\mathbf{X}} \right]} \quad (10)$$

357 where \mathbf{U}_c is the square diagonal matrix of order I of the membership degrees of cluster c ;
 358 $\bar{\mathbf{X}}$ is the centred “compromise” matrix (mean of the T data matrices \mathbf{X}_t); $\tilde{\mathbf{P}}$ is the weighted
 359 spatial matrix obtained as linear combination between the K proximity matrices as follows

$$\tilde{\mathbf{P}} = \sum_{k=1}^K w_k \mathbf{P}_k \quad (11)$$

360 where $0 \leq w_k \leq 1$ and $\sum_{k=1}^K w_k = 1$. The FM index (as the Moran’s index) ranges between
 361 -1 and 1. A value of 1 indicates perfect positive spatial autocorrelation, i.e. neighbouring
 362 units have similar values, 0 indicates no autocorrelation, i.e. units are spatially random
 363 located, and -1 indicates perfect negative spatial autocorrelation, i.e. neighbouring units
 364 have dissimilar values (Páez & Scott, 2005). Thus, the higher the FM value, the better
 365 the geographical assignment of the units to the clusters.
 366

367 Moreover, the Fuzzy Moran’s index, as the Moran’s index, can be interpreted as a mea-
 368 sure of spatial spill-over effect (Ma et al., 2015; Yang, 2012). In the literature, the spatial
 369 spill-over effect is considered as the indirect or unintentional effects that a geographical
 370 area exerts on other neighbour areas (Yang & Fik, 2014). A positive spill-over effect is
 371 obtained when an area benefits of their neighbours influence due to the existence of spatial
 372 externalities across area.

373 2.6. Some comparative assessment

374 Our proposal inherits all the advantages of the ingredients considered in the method-
 375 ological framework. In particular, in a comparative assessment point of view, with respect
 376 to some methods suggested in the literature we have the following evidences.

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- The fuzzy clustering methods proposed by D’Urso et al. (2018) show very good performance for clustering units with time-varying information. However, when the units are regions, geographical areas, etc., it is more useful to analyse this kind of units by considering clustering methods capable to capture the territorial nature of the units. To this purpose, the method proposed in this paper is able to cluster units not only considering time information but also taking into account additional information connected to spatial characteristics of the units. In particular, our method is able to cluster territorial units considering explicitly in the objective function the spatial information connected to the units—territorial proximity and spatial autocorrelation (see sections 2.2 and 2.3.2). Notice that, the fuzzy clustering methods proposed by D’Urso et al. (2018) could be applied to territorial units, but ignoring the territorial information that characterizes this type of unit. However, this would represent a relevant loss of information in the spatial analysis process. Furthermore, with respect to the fuzzy clustering methods suggested by D’Urso et al. (2018) based on the Euclidean distance, the proposed method inherits all the advantages of the DTW-based dissimilarity measure (see, section 2.1).
- The Fuzzy *C*-Means clustering method for spatial time series proposed by Coppi et al. (2010) (Cross-Sectional Fuzzy *C*-Means for Spatial-Temporal Trajectories, CS-FCM-STT) is able to cluster territorial units with time-varying information. With respect to this method our proposal has two more advantages inherited: (i) by the kind of prototypes utilized in our method (i.e. medoids vs centroids); (ii) by the characteristics of the spatial component considered in the objective function of the proposed method.
 - (i) With respect to the advantage connected to the kind of prototypes (i.e. medoids), adopting PAM approach, the prototypes of each cluster (medoids) are territorial units actually observed and not “virtual” territorial units like the “centroids” derived with a Fuzzy *C*-Means—as in the method suggested by Coppi et al. (2010). Overall, having non-fictitious representative territorial units available makes interpreting the obtained clusters easier, which is often very useful in geographical and territorial applications. In fact, “in many clustering problems one is particularly interested in a characterization of the clusters by means of typical or representative objects [territorial units]. These are objects [territorial units] that represent the various structural aspects of the set of objects [territorial units] being investigated. There can be many reasons for searching for representative objects [territorial units]. Not only can these objects [territorial units] provide a characterization of the clusters, but they can often be used for further work or research, especially when it is more economical or convenient to use a small set of k objects [C territorial units in our case] instead of the large set one started off with” (Kaufman & Rousseeuw, 2005). Furthermore, PAM clustering approach is slightly more robust than *C*-Means approach (Garcia-Escudero & Gordaliza, 1999; ?; Estivill-Castro & Yang, 2004; Kaufman & Rousseeuw, 2005), hence DTW-FCMd-STT is relatively more resistant to the presence of noise in the data than CS-FCM-STT.

419 (ii) With respect to the advantages connected to spatial dependent term of the ob-
 420 jective function, our spatial term is more general compared with the spatial term
 421 considered in the method suggested by Coppi et al. (2010). In fact, as remarked in
 422 section 2.3.2, it is capable to consider different level of spatial proximity (multilevel
 423 proximity) and then it is more informative in a spatial point of view in the sense that
 424 it is able to capture in deep the political and physical geographical characteristics
 425 -e.g. administrative and economic features and geophysical and orographic nuances-
 426 of the analysed territorial area. In this way, the spatial dependent term used in Coppi
 427 et al. (2010) is a particular case of the term adopted in our method. See section 2.3.2
 428 for more details.

429 3. Illustration with simulated data

430 3.1. Simulation study 1

431 In the following, a simulation study in which two contiguity matrices are considered for
 432 simplicity, is presented. The aim of this exercise is to assess the sensitivity of the clustering
 433 process to the contiguity matrices, according to the k -th spatial parameters β_k (formula
 434 4).

435 An artificial data set is generated with two natural clusters and two units close to each
 436 other and characterized by soft memberships to one of the two clusters. Two contiguity
 437 matrices, one with contiguity only among the units within the natural clusters (including
 438 the soft membership unit) and one including the contiguity between the soft membership
 439 units as well, are generated. The aim of the simulation is to verify the decreasing of the
 440 fuzzy membership degrees of the two soft membership units with respect to their natural
 441 clusters and, eventually, even their memberships to the same cluster while increasing the
 442 spatial penalty coefficient of the matrix including contiguity between them. For this reason,
 443 the spatial penalty coefficients β_1 and β_2 range in $(0, 8)$.

444 The number of units, variables, and periods of time considered are $I = 8$, $J = 2$, and
 445 $T = 6$, respectively. In the contiguity matrix \mathbf{P}_2 , two sets of contiguous units are defined,
 446 i.e. $(1, 2, 3, 4)$ and $(5, 6, 7, 8)$, whereas in \mathbf{P}_1 the contiguity between units 4 and 5 is
 447 added. The contiguity matrices \mathbf{P}_1 and \mathbf{P}_2 are the following:

$$\mathbf{P}_1 = \begin{pmatrix} & u1 & u2 & u3 & u4 & u5 & u6 & u7 & u8 \\ u1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ u2 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ u3 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ u4 & 1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 \\ u5 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 1 \\ u6 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 \\ u7 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 \\ u8 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 \end{pmatrix}$$

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$$\mathbf{P}_2 = \begin{pmatrix} & u1 & u2 & u3 & u4 & u5 & u6 & u7 & u8 \\ u1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ u2 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ u3 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ u4 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ u5 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 \\ u6 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 \\ u7 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 \\ u8 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 \end{pmatrix}$$

449 The generation process of the dataset is summarized in Table 1. The defined clusters
 450 are (1, 2, 3) and (6, 7, 8). Units 4 and 5 are characterized by a *fuzzy* membership to
 451 clusters (1, 2, 3) and (6, 7, 8), respectively. Going from data configuration 1) to data
 452 configuration 4), we can note that units 4 and 5 are getting closer and closer (Table 1 and
 453 Figure 3).

Configuration	units 1,2,3	unit 4	unit 5	units 6,7,8
1) $j=1$	$U[0.0, 0.5]$	$U[0.8, 1.0]$	$U[1.0, 1.2]$	$U[1.5, 2.0]$
$j=2$	$U[0.0, 0.5]$	$U[0.8, 1.0]$	$U[1.0, 1.2]$	$U[1.5, 2.0]$
2) $j=1$	$U[0.0, 0.5]$	$U[0.85, 1.0]$	$U[1.0, 1.15]$	$U[1.5, 2.0]$
$j=2$	$U[0.0, 0.5]$	$U[0.85, 1.0]$	$U[1.0, 1.15]$	$U[1.5, 2.0]$
3) $j=1$	$U[0.0, 0.5]$	$U[0.9, 1.0]$	$U[1.0, 1.1]$	$U[1.5, 2.0]$
$j=2$	$U[0.0, 0.5]$	$U[0.9, 1.0]$	$U[1.0, 1.1]$	$U[1.5, 2.0]$
4) $j=1$	$U[0.0, 0.5]$	$U[0.95, 1.0]$	$U[1.0, 1.05]$	$U[1.5, 2.0]$
$j=2$	$U[0.0, 0.5]$	$U[0.95, 1.0]$	$U[1.0, 1.05]$	$U[1.5, 2.0]$

Table 1: Data generation process for simulation study 1. Two clusters are generated from the data. Going from configuration 1) to configuration 4), units 4 and 5 are getting closer

454 The membership degree obtained in the case of the fourth data configuration (see Table
 455 1 and Figure 3) are reported in Table 2. By suitably tuning the values of β_1 and β_2 , and
 456 therefore the separate influence of the two contiguity matrices \mathbf{P}_1 and \mathbf{P}_2 , we can see how
 457 the two units 4 and 5 become more clearly separated, and then classified to the respective
 458 clusters when $\beta_1 < \beta_2$, or, on the contrary, are classified in the same cluster, when $\beta_1 > \beta_2$.

459 For more details on the membership degrees and on performance results, see the Ap-
 460 pendix Appendix A.1 to this paper.

461 3.2. Simulation study 2

462 This simulation study is similar to that presented in section 3.1. We increased the
 463 number of objects and of clusters, to show the performance of DTW-FCMd-STT in a
 464 more complex environment. Similarly as in an simulation study 1, artificial data set is
 465 generated with four natural clusters and four units close to each other characterized by
 466 soft membership to one of the four clusters. Two contiguity matrices, one with contiguity

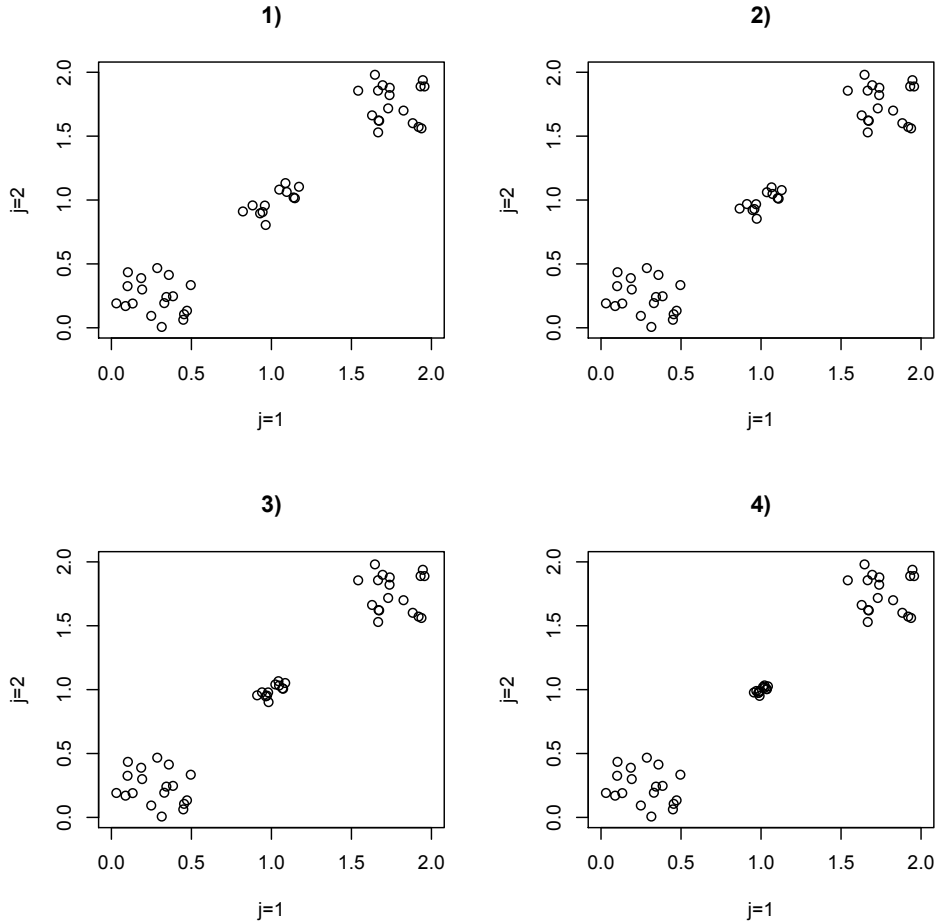


Figure 3: Data generation process for simulation study 1. Two clusters are generated from the data. Going from configuration 1) to configuration 4), units 4 and 5 are getting closer

(β_1, β_2)	(0, 0)		(4, 0)		(0, 4)		(8, 0)		(0, 8)	
cluster	1	2	1	2	1	2	1	2	1	2
1	0.9999	0.0001	0.9999	0.0001	0.9999	0.0001	0.9999	0.0001	0.9999	0.0001
2	0.9999	0.0001	0.9999	0.0001	0.9999	0.0001	0.9999	0.0001	0.9999	0.0001
3	1.0000	0.0000	1.0000	0.0000	1.0000	0.0000	1.0000	0.0000	1.0000	0.0000
4	0.6271	0.3729	0.6853	0.3147	0.6689	0.3311	0.7168	0.2832	0.7051	0.2949
5	0.4874	0.5126	0.5256	0.4744	0.4603	0.5397	0.5169	0.4831	0.4138	0.5862
6	0.0000	1.0000	0.0000	1.0000	0.0001	0.9999	0.0000	1.0000	0.0001	0.9999
7	0.0000	1.0000	0.0000	1.0000	0.0000	1.0000	0.0000	1.0000	0.0000	1.0000
8	0.0003	0.9997	0.0001	0.9999	0.0004	0.9996	0.0001	0.9999	0.0004	0.9996

Note: Medoids' membership degrees are in bold.

Table 2: Membership degrees for simulation study 1 obtained under the data configuration 4), according to different combinations of β_1 and β_2

only among the units within the natural clusters (including the soft membership unit) and one including the contiguity among the soft membership units as well, are generated. The aim of the simulation is to verify the decreasing of the fuzzy membership degree of the four soft membership units to the natural clusters and eventually even their membership to the same cluster while increasing the spatial penalty coefficient of the matrix including contiguity among them. To this end, the spatial penalty coefficients β_1 and β_2 range in $(0, 20)$.

The number of units, variables, and periods of time considered are $I = 16$, $J = 2$, and $T = 6$, respectively. In the first contiguity matrix (\mathbf{P}_2), the contiguous units are (1, 2, 3, 4), (5, 6, 7, 8), (9, 10, 11, 12) and (13, 14, 15, 16), whereas in \mathbf{P}_1 the contiguity among units 4, 5, 12, 13 is added.

The generation process of the dataset is summarized in Table 3. The defined clusters are (1, 2, 3), (6, 7, 8), (9, 10, 11), (14, 15, 16). Units 4, 5, 12, 13 are characterized by a *fuzzy* membership to clusters (1, 2, 3), (6, 7, 8), (9, 10, 11), (14, 15, 16), respectively. Going from data configuration 1) to data configuration 4) units 4, 5, and 12, 13 are getting closer and closer, respectively (Table 3 and Figure 4).

Configuration	units 1,2,3	unit 4	unit 5	units 6,7,8	units 9,10,11	unit 12	unit 13	units 14,15,16
1) $j=1$	$U[0.0, 0.5]$	$U[0.6, 0.7]$	$U[0.6, 0.7]$	$U[0.0, 0.5]$	$U[1.5, 2.0]$	$U[1.3, 1.4]$	$U[1.3, 1.4]$	$U[1.5, 2.0]$
$j=2$	$U[0.0, 0.5]$	$U[0.6, 0.7]$	$U[1.3, 1.4]$	$U[1.5, 2.0]$	$U[1.5, 2.0]$	$U[1.3, 1.4]$	$U[0.6, 0.7]$	$U[0.0, 0.5]$
2) $j=1$	$U[0.0, 0.5]$	$U[0.7, 0.8]$	$U[0.7, 0.8]$	$U[0.0, 0.5]$	$U[1.5, 2.0]$	$U[1.2, 1.3]$	$U[1.2, 1.3]$	$U[1.5, 2.0]$
$j=2$	$U[0.0, 0.5]$	$U[0.7, 0.8]$	$U[1.2, 1.3]$	$U[1.5, 2.0]$	$U[1.5, 2.0]$	$U[1.2, 1.3]$	$U[0.7, 0.8]$	$U[0.0, 0.5]$
3) $j=1$	$U[0.0, 0.5]$	$U[0.8, 0.9]$	$U[0.8, 0.9]$	$U[0.0, 0.5]$	$U[1.5, 2.0]$	$U[1.1, 1.2]$	$U[1.1, 1.2]$	$U[1.5, 2.0]$
$j=1$	$U[0.0, 0.5]$	$U[0.8, 0.9]$	$U[1.1, 1.2]$	$U[1.5, 2.0]$	$U[1.5, 2.0]$	$U[1.1, 1.2]$	$U[0.8, 0.9]$	$U[0.0, 0.5]$
4) $j=1$	$U[0.0, 0.5]$	$U[0.9, 1.0]$	$U[0.9, 1.0]$	$U[0.0, 0.5]$	$U[1.5, 2.0]$	$U[1.0, 1.1]$	$U[1.0, 1.1]$	$U[1.5, 2.0]$
$j=2$	$U[0.0, 0.5]$	$U[0.9, 1.0]$	$U[1.0, 1.1]$	$U[1.5, 2.0]$	$U[1.5, 2.0]$	$U[1.0, 1.1]$	$U[0.9, 1.0]$	$U[0.0, 0.5]$

Table 3: Data generation process for simulation study 2. Four clusters are generated from the data. Going from configuration 1) to configuration 4), units 4, 5, and 12, 13 are getting closer

Once again, according to the combination of β_1 and β_2 , the *fuzzy* units get more separated when $\beta_1 < \beta_2$, while eventually are classified in the same cluster when $\beta_1 > \beta_2$.

For more details on the membership degrees and on performance results, see the Appendix Appendix A.2 to this paper.

3.3. Simulation study 3

In this simulation study we highlight two main features of the proposed clustering method:

1. the capability to deal with time series of different length;
2. the capability to fully exploit spatial information.

We simulated a dataset of 20 three-variate ($I = 20$, $J = 3$) time series of length ranging from $T = 6$ to $T = 10$. The data generation process yielded to three partially overlapping clusters ($C = 3$) of size 10, 5 and 5, respectively (see Figure 5).

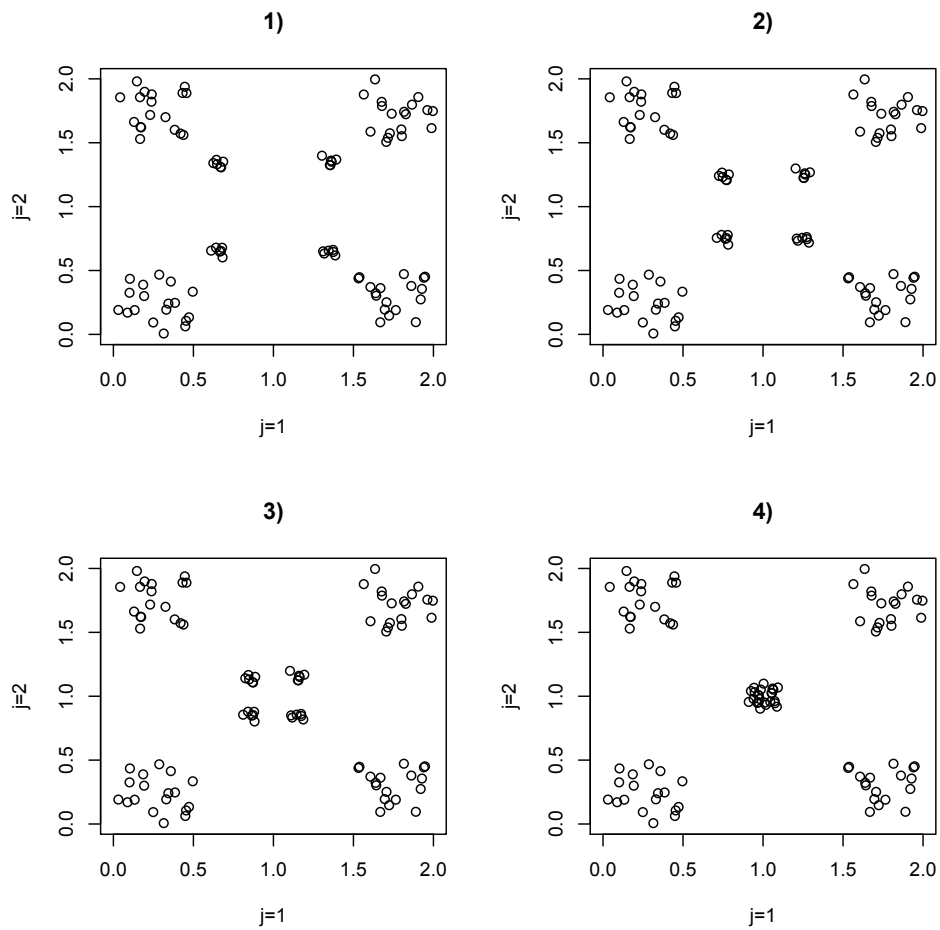


Figure 4: Data generation process for simulation study 2. Four clusters are generated from the data. Going from configuration 1) to configuration 4), units 4, 5, and 12, 13 are getting closer

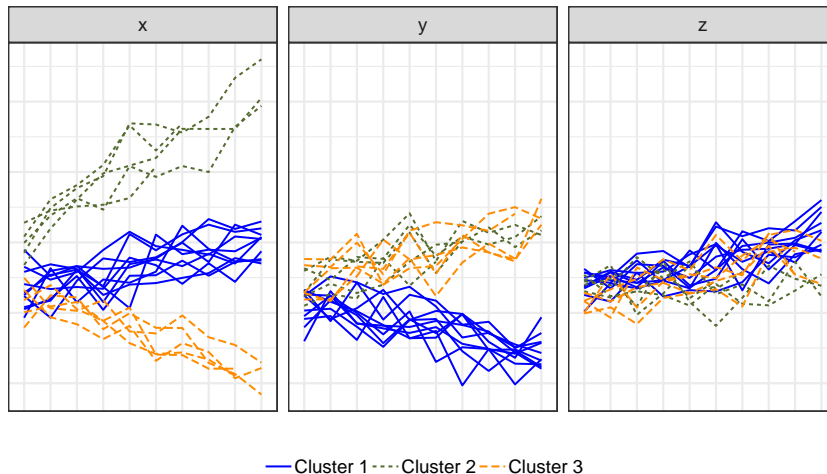


Figure 5: Simulated data for simulation study 3. Data are generated to be classified into three partially overlapping clusters. Time series belonging to different clusters are depicted with different colours and line types

495 As for the spatial dependence, we generated two proximity matrices, \mathbf{P}_1 and \mathbf{P}_2 , illus-
 496 trated in Figure 6. A black square indicate that there is some kind of proximity between i
 497 and j . The two matrices refer to different notions of proximity, which are closely related to
 498 those observed in the empirical application: \mathbf{P}_1 refers to a situation in which two units are
 499 neighbours if they share a border; \mathbf{P}_2 represents a situation in which proximity is due to
 500 the fact that belong to the same macro-area, even if they are not neighbour. Furthermore,
 501 each macro-area corresponds to a different cluster. By observing \mathbf{P}_1 and \mathbf{P}_2 , there are some
 502 units that are neighbours even if they belong to different macro-areas, and some units that
 503 belong to the same macro-area but they are not neighbour. Finally, the parameters β_1 and
 504 β_2 are set to 0 or 1.8, depending on how the spatial information is exploited.

505 The purpose of the present simulation is to show the capability of DTW-FCMd-TSS
 506 to individuate the three clusters, even if data are rather noise, by exploiting the spatial
 507 information. For comparison's sake we consider four cases, described in Table 4. The first
 508 case refers to DTW-FCMd clustering method described in D'Urso et al. (2018). The second
 509 and the third cases are particular instances of the proposed DTW-FCMd-STT, in which
 510 we exploited only a part of the spatial information provided by the proximity matrices P_1
 511 and P_2 (see Figure 6). In the fourth case, the spatial information is fully exploited.

512 To evaluate the classification capability, we used the Fuzzy Rand Index (FRI) proposed
 513 by Hüllermeier et al. (2012), comparing the fuzzy partition obtained with the theoretical
 514 crisp reference partition. The closer FRI is to 1, the closer the fuzzy partition to the
 515 theoretical crisp reference partition. The results of the simulation are reported in the last
 516 column of Table 4. DTW-FCMd provides a partition that takes into account only the
 517 time dimension, which is rather fuzzy as explained, thus explaining the relative low value
 518 of FRI (case A). Exploiting only a part of the spatial information slightly enhances the
 519 classification capability of DTW-FCMd-STT with respect to DTW-FCMd (cases B and

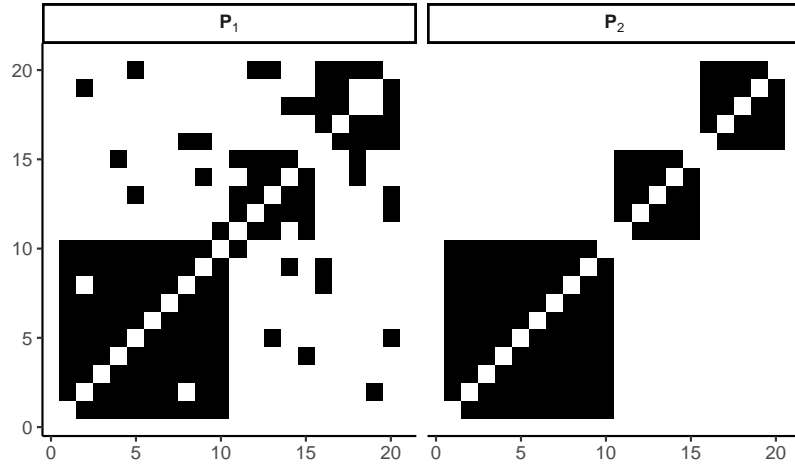


Figure 6: Proximity matrices – black squares indicate the proximity between two generic units (simulation study 3)

Case	Method	P_1	P_2	β_1	β_2	FRI
A	DTW-FCMd	No	No	0.0	0.0	0.720
B	DTW-FCMd-STT	Yes	No	1.8	0.0	0.734
C	DTW-FCMd-STT	No	Yes	0.0	1.8	0.741
D	DTW-FCMd-STT	Yes	Yes	1.8	1.8	0.985

Table 4: Fuzzy Rand Indices for simulation study 3, according to different clustering models (row wise) and different settings of spatial parameters (column wise)

520 C). On the contrary, by exploiting the whole spatial information, the clustering method
 521 is capable to correctly identify the clustering structure of the data at hand, properly in-
 522 corporating the spatial information (case D). This evidence is further corroborated by the
 523 membership degrees obtained in the four cases, illustrated by the ternary plots¹ reported
 524 in Figure 7. In the ternary plot, every point represents the membership degrees of the
 525 corresponding time series in the three cluster. The more a point is close to a vertex of
 526 the triangle, the less uncertain is the assignment of the time series to the corresponding
 527 cluster.

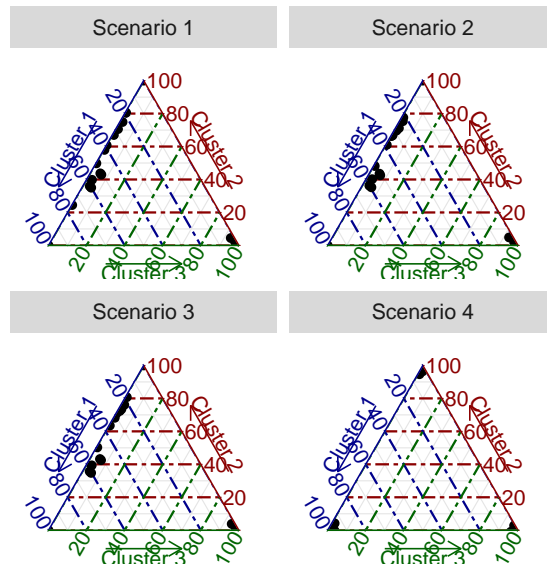


Figure 7: Membership degrees (simulation study 3)

528 As a final word, it should be stressed that the purpose of the present simulation is to
 529 clarify how the spatial information is embedded into the proposed clustering method.

530 3.4. Simulation study 4

531 For this simulation study, we partly replicated a simulation study proposed by D’Urso
 532 (2005a) and D’Urso et al. (2018) with an artificial dataset characterised by three well-
 533 separated clusters of four, three, and three multivariate time trajectories, respectively, and
 534 one outlier time trajectory (Figure 8). The length of each time series simulated is $T = 6$.
 535 The proximity matrix in Figure 9 represents the spatial component that has been included
 536 in this simulation study. Notice that a black square indicates proximity between units i
 537 and i' , while a red square indicates proximity between an outlier and a generic unit.

538 Being the time series of the same length and having added only one proximity matrix,
 539 DTW-FCMD (D’Urso et al., 2018), our proposed clustering method (DTW-FCMd-STT),
 540 CS-FCM (D’Urso, 2005a), and CS-FCM-STT (Coppi et al., 2010) are fully comparable.

¹The ternary plots have been produced by means of the R package `ggtern` (Hamilton & Ferry, 2018).

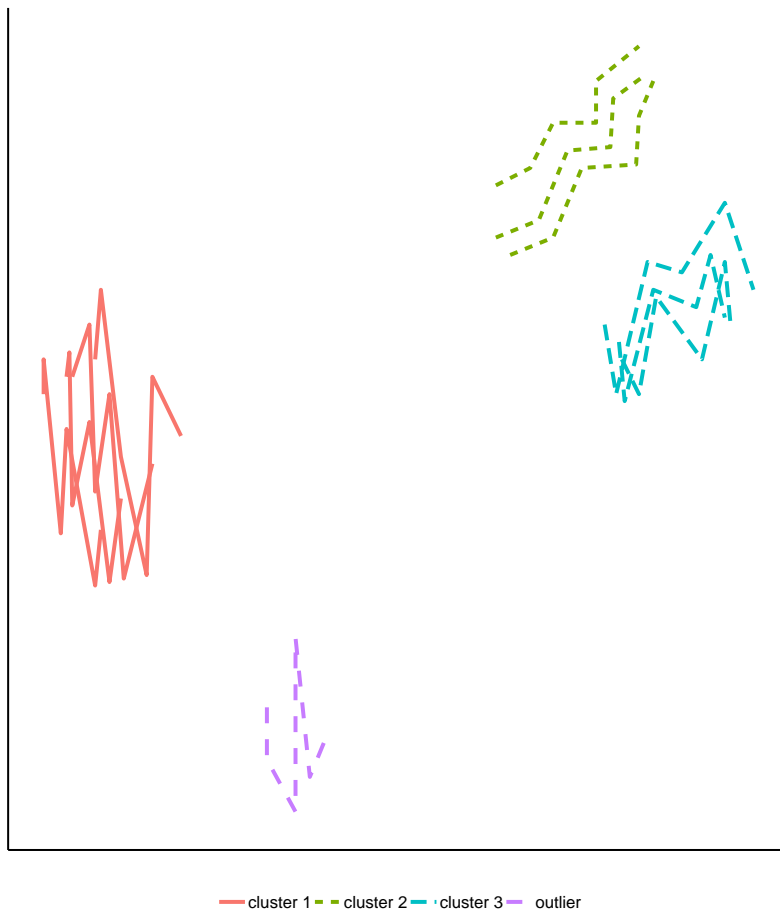


Figure 8: Simulated data for simulation study 4. Data are generated to be classified into three well separated clusters and one outlier time series. Time series belonging to different clusters and the outliers are depicted with different colours and line types

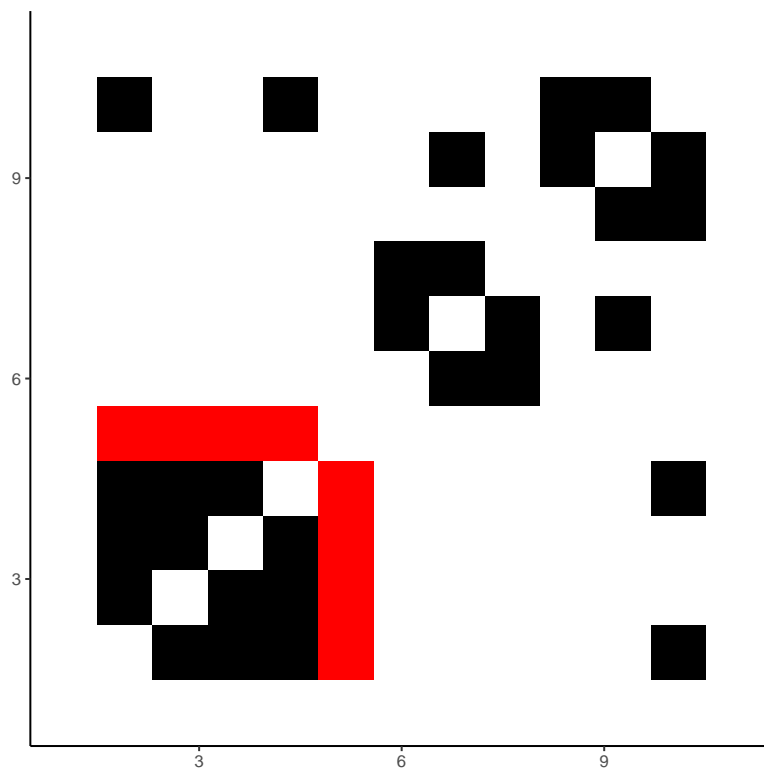


Figure 9: Proximity matrix – black squares indicate the proximity between two generic units: red squares indicate the proximity between the outlier and the corresponding unit (simulation study 4)

Case	Method	Outlier	Spatial information	<i>FRI</i>
A	DTW-FCMd	No	No	0.984
B		Yes	No	0.797
C	DTW-FCMd-STT	No	Yes	0.978
D		Yes	Yes	0.978
E	CS-FCM	No	No	0.990
F		Yes	No	0.780
G	CS-FCM-STT	No	Yes	0.948
H		Yes	Yes	0.761

Table 5: Fuzzy Rand Indices for simulation study 4, according to different clustering models (row wise) and to the presence of spatial information and/or the outlier time series (column wise)

Therefore, the simulation study is aimed to compare the classification capability of the above mentioned methods. Implicitly, we also compare DTW-FCMd-STT and CS-FCM-STT in the way they exploit the spatial information, in particular in the presence of a slight disturbance, given by the outlier time series. The value of β for both DTW-FCMd-STT and CS-FCM-STT has been set to 1.

In Table 5, *FRI* values for the different cases examined are reported. As expected, when the outlier time series is dropped from data, all clustering methods display a very good clustering performance. On the contrary, only DTW-FCMD-STT is able to resist to the presence of one outlier in the dataset.

4. Illustration with economic data

4.1. Study data

In this analysis, we consider annual tourist arrivals in the municipalities located in South-Tyrol region (Northern Italy) collected by ASTAT (the local institute of statistics) from 2008 to 2014. Given a geographic region having various localities as possible tourist attractions, we aim at identifying agglomerations of cities characterised by a common trend of the tourist flows over time taking into account the particular geographical and political underlined structure. South-Tyrol is in fact a tourist destination characterised by 116 municipalities grouped into eight administrative districts that follow the geomorphology of the region (see Figure 10).

Therefore, each municipality is characterised by two spatial information: whether two units are contiguous or not; whether two units belong to the same district or not. In this paper, each municipality is described by the annual time series on tourist flows from the two main markets, i.e. Germany and Italy (domestic tourists). Table 6 shows the descriptive characteristics of the two time series highlighting the high variability of arrivals among municipalities in each year observed.

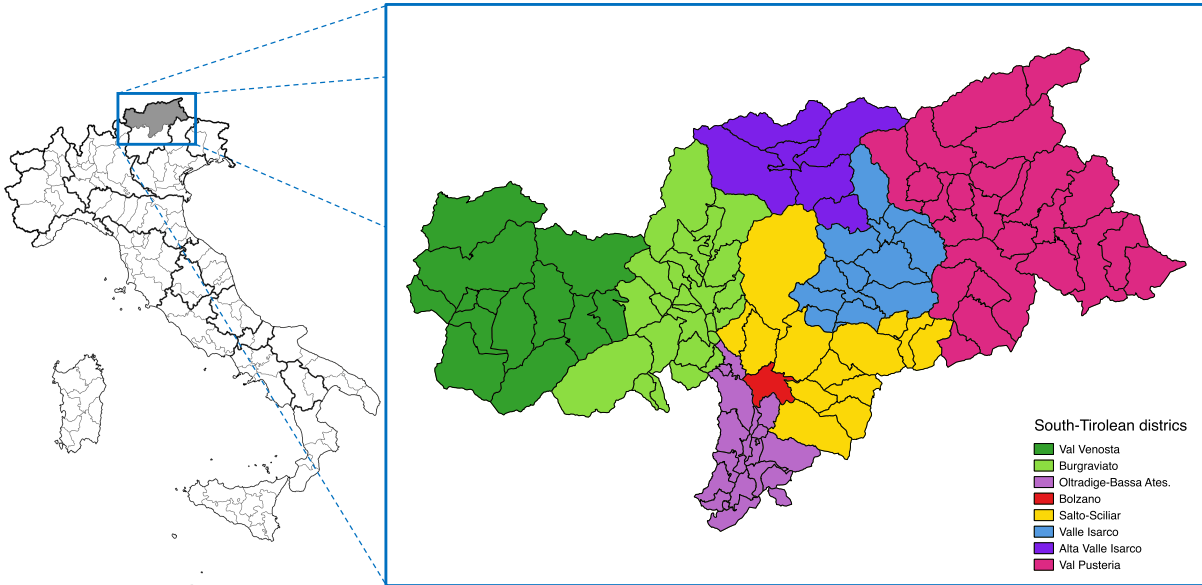


Figure 10: South-Tyrol region

Year	Mean		SD		MIN		MAX	
	Germany	Italy	Germany	Italy	Germany	Italy	Germany	Italy
2008	19843.34	18198.87	20058.15	25493.66	0	0	103026	109185
2009	20334.71	18849.07	20735.57	26094.45	0	0	106228	113199
2010	21005.07	18997.12	21771.90	26757.23	0	2	111202	115211
2011	21901.66	18952.86	22375.17	26338.25	0	2	114095	112591
2012	23066.78	18774.24	23464.45	25751.07	0	2	117825	113070
2013	23300.02	18188.68	23779.26	25245.33	0	3	117064	110082
2014	23889.45	18024.78	23973.20	24675.21	0	0	111843	111070

Table 6: Descriptive statistics of annual tourist arrivals from Germany and Italy

566 As highlighted in Figure 11, units are spatially autocorrelated, especially with regards
 567 to domestic tourists who are mainly grouped in Val Pusteria (East part of the region).

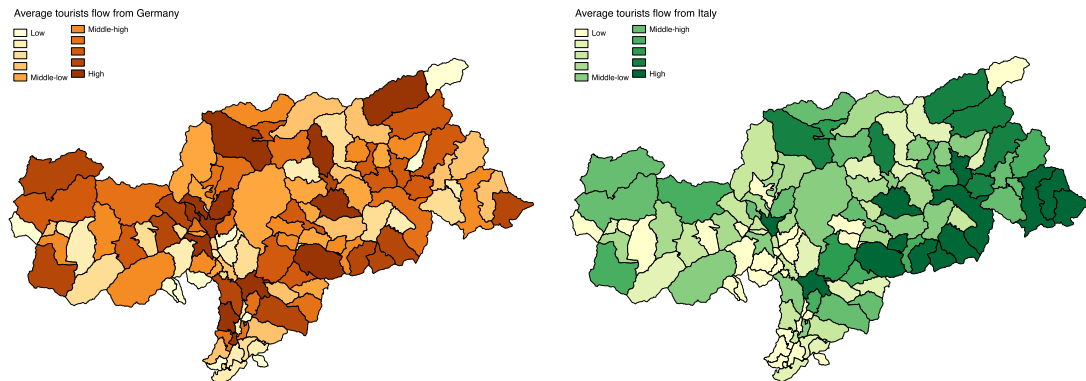


Figure 11: Average annual tourist flows

568 By means of the suggested DTW-FCMd-STT clustering algorithm with spatial penalty
 569 terms, we have the opportunity to: 1) identify agglomerations of cities characterised by
 570 similar tourist arrival trends, by considering units' geographical proximity and district
 571 memberships; 2) recognise the medoid of each agglomeration, i.e. the municipality that
 572 characterises each agglomeration and that can be considered as the representative touristic
 573 municipality (in statistical terms) of a given sub-region.

574 4.2. Clustering results

575 The optimal iterative solution is obtained by solving the DTW-FCMd-STT algorithm
 576 with the Lagrangian multipliers method where:

- 577 (1) the fuzziness parameter has been fixed to $m = 1.5$ (Kamdar & Joshi, 2000);
- 578 (2) the optimal number of clusters C of the DTW-FCMd-STT algorithm without penalty
 579 terms has been identified by means of the fuzzy cluster validity measures presented in
 580 section 2.4;
- 581 (3) the values of the two spatial penalty coefficients (i.e. β_1 and β_2) have been selected
 582 in order to maximize the multivariate spatial autocorrelation of the whole area (with-
 583 out considering the possible clustering structure) when both proximity matrices are
 584 considered.

585 Figure 12 summarises the values of the FS and XB indices calculated for any partition
 586 C from 2 to 9 when the spatial penalty terms are not included in the WTD-FCMd clustering
 587 algorithm. The trajectories of the two indices suggest that the best partitions are $C = 2$
 588 followed by the four and six clusters partitions.

589 The weighted multivariate spatial autocorrelation of the whole area has been computed
 590 by means of equation 10 imposing $\bar{\mathbf{X}}$ equals to the identity matrix. The weighting spatial
 591 matrix $\tilde{\mathbf{P}}$ is computed through equation 11 fixing $K = 2$:

$$\tilde{\mathbf{P}} = w_1 \mathbf{P}_1 + w_2 \mathbf{P}_2$$

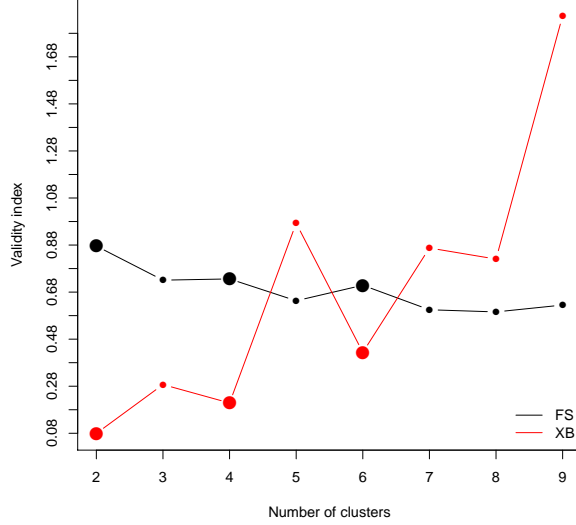


Figure 12: *FS* and *XB* validity index values for each cluster partition C from 2 to 9

592 where \mathbf{P}_1 is a non-negative (116×116) data matrix, whose generic entry $p_{1ii'}$ can be
593 interpreted as the spatial proximity between the i -th and i' -th units ($i, i' = 1, \dots, 116$), \mathbf{P}_2
594 is another non-negative (116×116) data matrix, whose generic entry $p_{2ii'}$ describes whether
595 the i -th and i' -th units belong to the same district or not, $w_1 = 1 - w_2$ is the parameter
596 to be identified in order to maximize the weighted multivariate spatial correlation. Once
597 the optimal value of w_1 , i.e. w_1^* , is identified, we suggest to define the two spatial penalty
598 parameters, i.e. β_1 and β_2 , such as $w_1 = \frac{\beta_1}{\beta_1 + \beta_2}$. Consequently, the best combination
599 of β_1 and β_2 will be the one that allows to obtain the closer value to w_1^* . In this way
600 we guarantee that the higher w_1 , the higher β_1 , i.e. the two parameters related to the
601 same proximity matrix \mathbf{P}_1 go on the same direction. In this study, the maximum value
602 of the weighted multivariate spatial autocorrelation for the whole area is 0.21, indicating
603 a positive spatial autocorrelation between observed municipalities in inbound tourist from
604 Germany and domestic tourist flows, and $w_1^* = 0.68$, as represented in Figure 13.

605 In the following, we will concentrate our attention on the four-clusters and six-clusters
606 solutions. In fact, from a managerial and practical perspective, the two-clusters is not an
607 appealing solution since it is not generally informative and useful to draw new policies and
608 strategies.

609 Fixing $C = 4$, the best combination of β_1 and β_2 , i.e. the one that allows to maximize
610 the weighted multivariate spatial autocorrelation, is $\beta_1 = 0.01$ and $\beta_2 = 0.005$, which
611 allows to obtain a fairly high spatial autocorrelation between geographical units ($FM =$
612 0.50). Comparing the final 4 clusters obtained with and without the two spatial proximity
613 matrices, it emerges that the spatial information allows making small adjustments to the
614 membership degrees of the final matrix but not severe changes in the final fuzzy cluster
615 partition.

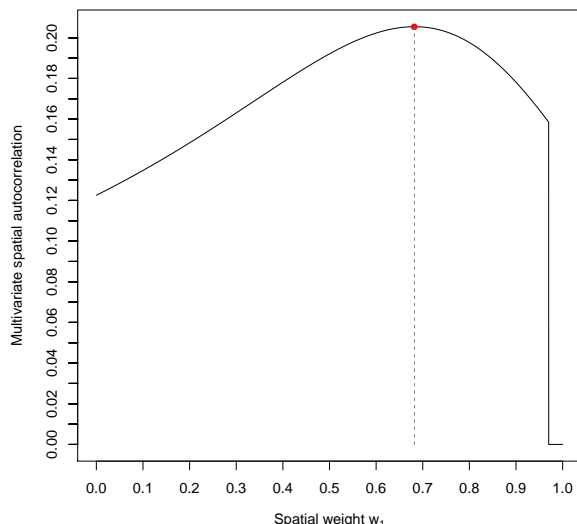


Figure 13: Values of the multivariate spatial autocorrelation of the whole area when proximity matrices are considered

616 Conversely, when $C = 6$ the best combination of β_1 and β_2 is $\beta_1 = 0.61$ and $\beta_2 = 0.32$,
 617 which allows to obtain a fairly high spatial autocorrelation between geographical units
 618 ($FM = 0.47$). As in the previous configuration, the proximity between areas is more
 619 relevant than the belonging to the same district. Figure 14 compares the membership
 620 degrees of each unit computed using DTW-FCMd-STT with and without penalty terms.
 621 The most evident changes, both in terms of intensity and frequency, are observable in
 622 cluster 1, 4, and 5. A similar conclusion can be reached observing the fuzzy cluster size,
 623 i.e. the sum of membership degrees per cluster, represented in Table 7. This measure is
 624 a proxy of the cluster size usually gather from crisp algorithm and it allows to spot both
 625 niches (as cluster 2 and 6) and bigger clusters (as cluster 4 and 5). Overall, cluster 1, 4,
 626 and 5 are the biggest clusters that highlight also the biggest changes.

	1	2	3	4	5	6
Without spatial terms	10.7047	6.22686	9.02877	60.9413	22.6855	6.41291
With spatial terms	11.5986	6.19582	9.04499	61.2298	21.5608	6.37000

Table 7: Sum of the membership degrees by cluster

627 For a deeper understanding and interpretation of the differences between the results
 628 of the two clustering algorithms, the membership degrees of each town/village, along with
 629 the medoids of each cluster, are represented in Figure 15.

630 The final membership degrees to cluster 1, 4, and 5 obtained excluding and including
 631 the penalty terms are compared to point out the most relevant changes. It is worthy of

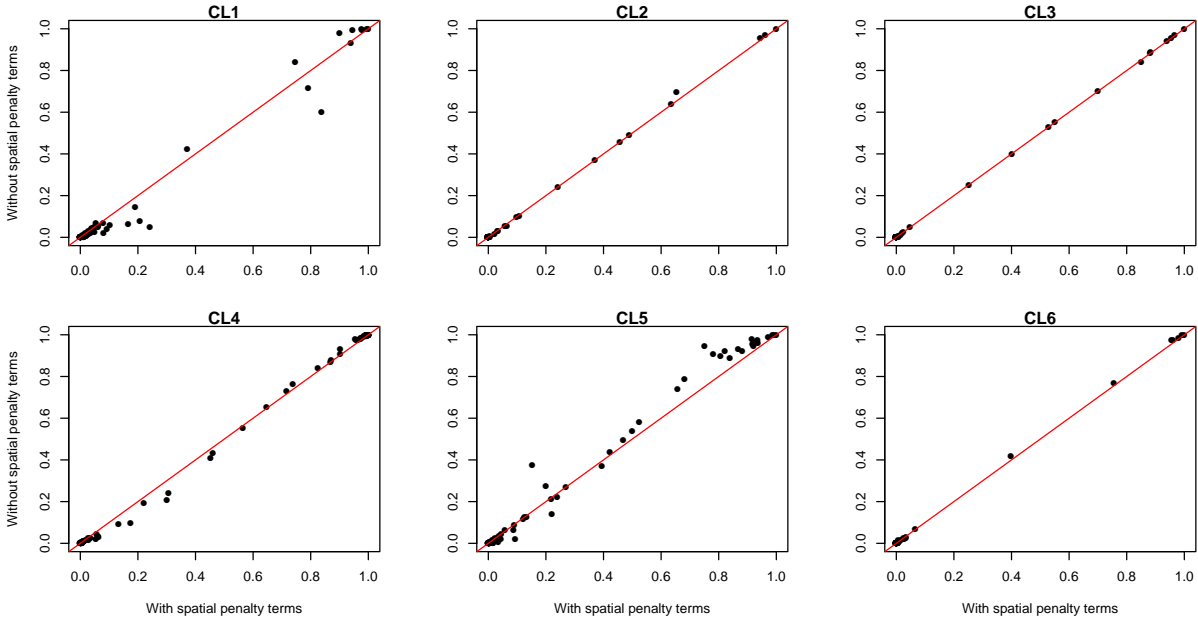


Figure 14: Comparing unit membership degrees to each cluster obtained using DTW-FCMd-STT with and without spatial terms

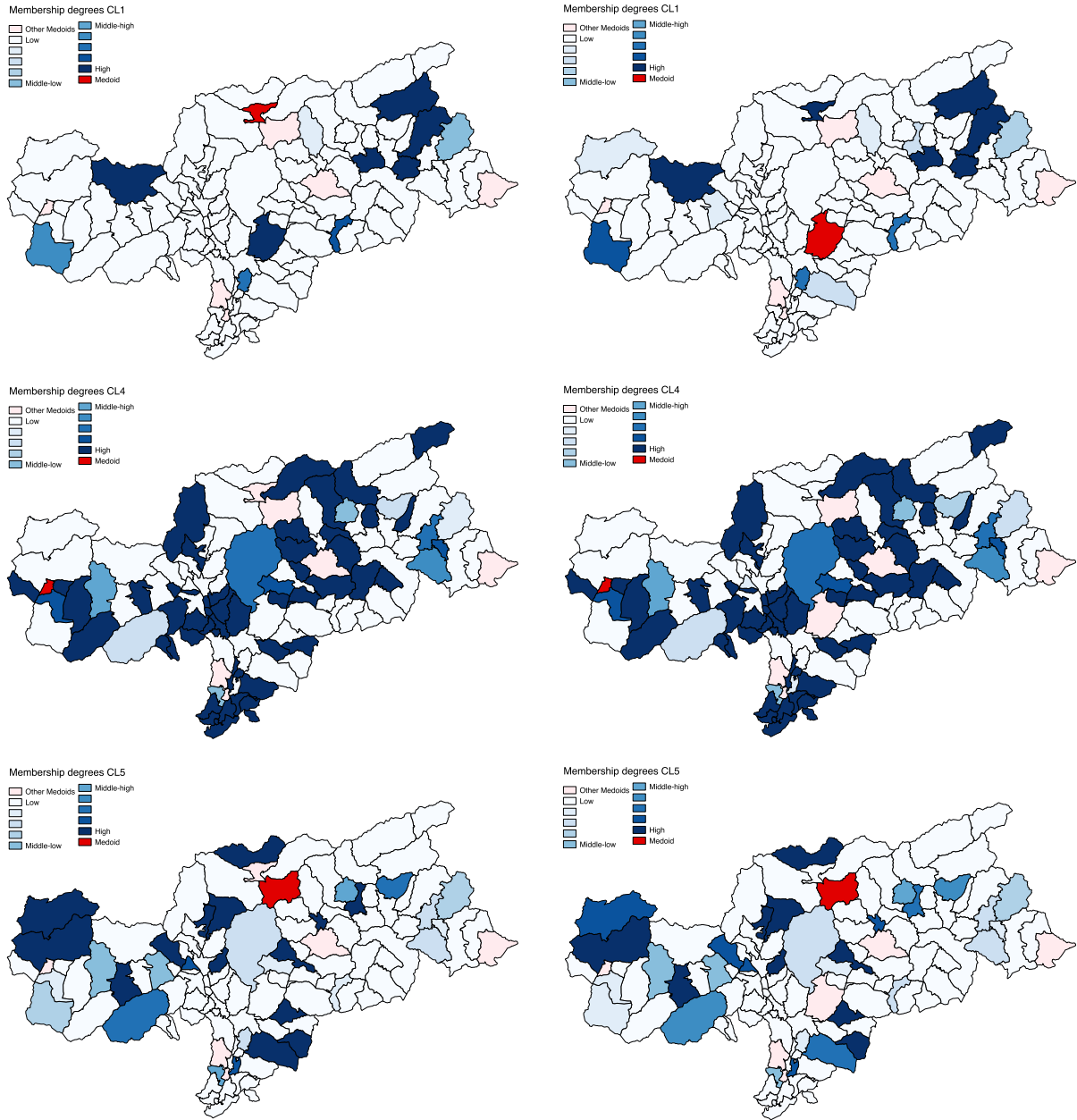
632 notice that the inclusion of the penalty terms in the clustering algorithm does not force
 633 final clusters to be made by neighbours town/village or to recall the districts. The change
 634 in the medoid of cluster 1 is the most noticeable and important change observable. This
 635 result have important practical consequences when policies and strategies are made at an
 636 aggregate (medoid) level instead of at a municipality (geographical unit) level.

637 For instance, marketing and promotional strategies to attract and host domestic or
 638 German tourists will be different depending on the decision to include or not the penalty
 639 terms (see Figure 16a). Furthermore, in Figure 16b the average cluster time series of the
 640 tourist flows coming from Germany and Italy are represented. Tourist flows are unchanged
 641 (domestic tourist) or slightly change (tourist from Germany) for cluster 2, 3, and 6, while
 642 the remaining clusters present more consistent variations, especially for tourists coming
 643 from Germany.

644 Therefore, due to the particular geographical and political structure of the region,
 645 ignoring the two proximity levels may lead to incorrect results and policies.

646 5. Conclusions

647 In this paper, the Dynamic Time Warping Fuzzy C -Medoids for Spatial-Temporal Tra-
 648 jectories (DTW-FCMd-STT) clustering algorithm with penalty terms, a new clustering
 649 algorithm for the classification of units described by both multivariate time series and spa-
 650 tial information, has been introduced. In particular, the main aim of this study is to present
 651 a multivariate generalisation of the Coppi et al. (2010) clustering algorithm by 1) adopting
 652 a more flexible distance measure, the DTW dissimilarity measure, and 2) extending the

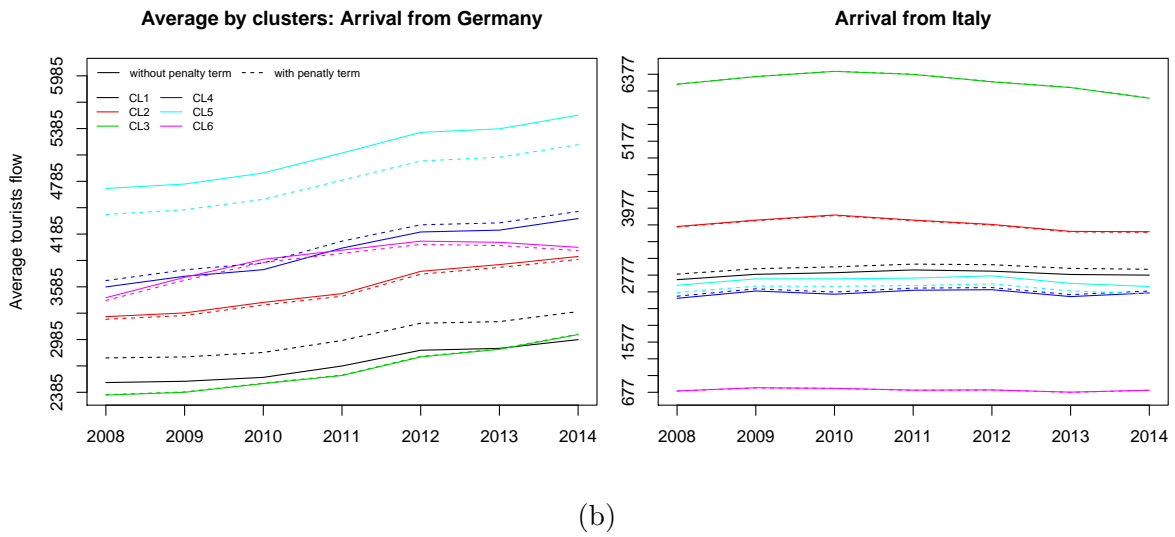
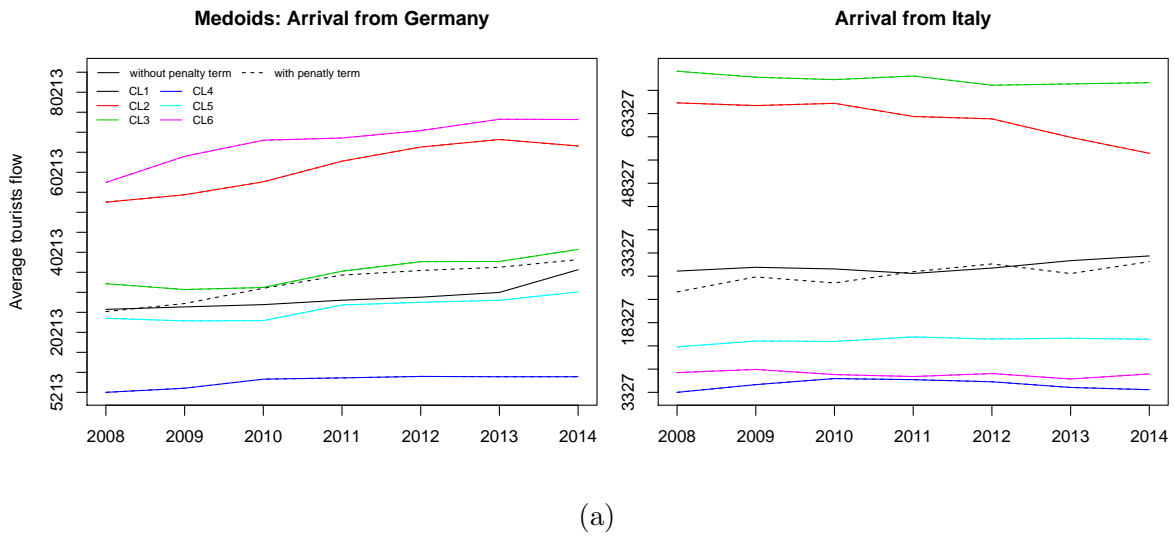


(a) Without spatial terms

(b) With spatial terms

Figure 15: DTW-FCMd-STT without (on the left) and with (on the right) spatial terms when $C = 6$

Figure 16: Medoids time series (16a) and weighted average arrivals by cluster (16b)



653 possibility to classify units on which either different kinds or different levels of proximity
654 are identifiable. Furthermore, a new weighted multivariate spatial autocorrelation index
655 to evaluate the autocorrelation of the final fuzzy partition, i.e. the Fuzzy Moran's index,
656 has been defined and presented.

657 Different simulation studies and a real dataset drawn by the tourism field have been
658 presented to illustrate the usefulness and effectiveness of the suggested clustering method
659 for spatial-temporal series. In particular, the findings of the simulation studies describe
660 the sensitivity of the DTW-FCMd-STT clustering algorithm to changes in the proxim-
661 ity matrices. The application to the real case study shows that the DTW-FCMd-STT
662 algorithm may help in the identification of groups that are spatially close, making more
663 appealing the applicability of the results of the cluster analysis. Furthermore, the Fuzzy
664 Moran's index reveal that a fairly high spatial autocorrelation between geographical units
665 exists. Consequently, this result also indicate the presence of a positive spill-over effect
666 among municipalities, i.e. one municipality's tourism industries affects the tourism flows
667 of neighbours municipalities due to the existence of spatial externalities.

668 Finally, it is worth exploring also the possibility of obtaining more robust version of
669 the proposed clustering algorithm, in order to cope with the presence of noise both in the
670 time and in the spatial dimensions.

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909 **Appendix A. Simulation studies**

910 *Appendix A.1. Simulation study 1*

911 In this section, we report some further comments on the first simulation study.

912 The medoids and the fuzzy membership obtained are illustrated in Table A.8. The
913 medoids' membership degrees are highlighted in bold. As we can observe, the medoids are
914 units 3 and 7 over all the data configurations. Furthermore, in each data configuration
915 the membership degrees of units 4 and 5 to each cluster decrease or increase alternating
916 the greater weight between the contiguity matrices \mathbf{P}_1 and \mathbf{P}_2 . In data configuration 4),
917 where units 4 and 5 are closest, units 5 is in the same cluster of unit 4 when the weight of
918 \mathbf{P}_1 is greater than the weight of \mathbf{P}_2 ($\beta_1 = 4$ and $\beta_2 = 0$; $\beta_1 = 8$ and $\beta_2 = 0$); in different
919 clusters when the weight of \mathbf{P}_2 is greater than the weight of \mathbf{P}_1 ($\beta_1 = 0$ and $\beta_2 = 4$; $\beta_1 = 0$
920 and $\beta_2 = 8$). In data configuration 4) when $\beta_1 = 8$ and $\beta_2 = 0$ the clusters are (medoid
921 in bold) (1, 2, **3**, 4, 5) and (6, **7**, 8); when $\beta_1 = 0$ and $\beta_2 = 8$ the clusters are (medoid in
922 bold) (1, 2, **3**, 4) and (5, 6, **7**, 8).

923 The performance of the proposed clustering method measured by the Fuzzy Silhouette
924 index FS —is described in Table A.9. As it can be seen, going from configuration 1) to 4)
925 the value of the silhouette increases. In fact the medoids remain the same (3 and 7) and
926 the *fuzzy* units 4 and 5 decrease their membership to the natural clusters (1, 2, 3) and
927 (7, 8, 9).

928 *Appendix A.2. Simulation study 2*

929 In this section, we report some further comments on the second simulation study.

930 The medoids and the fuzzy membership are illustrated in Tables A.10 and A.11. As
931 we can observe, the medoids are units 3, 7, 9, 14 over the data configurations 1) and 2);
932 units 4, 5, 12, 13 over almost all the data configurations 3) and 4). Table A.10 and A.11
933 show that in each data configuration the membership degrees of units 4, 5, 12, 13 to each
934 cluster decrease or increase alternating the greater weight between \mathbf{P}_1 and \mathbf{P}_2 . In data
935 configuration 3), where units 4, 5, 12, 13 are getting closer: 1) when $\beta_1 = 20$ and $\beta_2 = 0$
936 the units 4, 5, 12, 13 are in the same cluster and the clusters are (medoid in bold): (1, 2,
937 **3**), (6, **7**, 8), (4, 5, 9, 10, 11, **12**, 13), (**14**, 15, 16); 2) when $\beta_1 = 0$ and $\beta_2 = 20$ the units
938 4, 5, 12, 13 are in different clusters and the clusters are (medoid in bold) (1, 2, **3**, 4), (5,
939 6, **7**, 8), (**9**, 10, 11,12), (13, **14**, 15, 16).

940 In Table A.12 the main conclusions of the simulation study are reported. Notice that,
941 going from configuration 1), 2) to 3), 4), the value of the silhouette decreases. In configu-
942 rations 1), 2) the medoids are 3, 7, 9, 14; in configurations 3), 4) the medoids are almost
943 always 4, 5, 12, 13 (the *fuzzy* units). The performances get worse in data configuration
944 3) and 4) in relation to the increased similarity of the fuzzy units 4, 5, 12, 13. The best
945 performance in data configuration 3) is $(\beta_1, \beta_2) = (20, 0)$ where the medoids are 3, 7, 12,
946 14 and the high weight of \mathbf{P}_1 constraints the four fuzzy units in the same cluster (medoid
947 12).

(β_1, β_2)	(0, 0)		(4, 0)		(0, 4)		(8, 0)		(0, 8)	
	Data configuration 1)									
cluster	1	2	1	2	1	2	1	2	1	2
1	0.9999	0.0001	0.9999	0.0001	0.9999	0.0001	0.9999	0.0001	0.9999	0.0001
2	0.9999	0.0001	0.9999	0.0001	0.9999	0.0001	0.9999	0.0001	0.9999	0.0001
3	1.0000	0.0000	1.0000	0.0000	1.0000	0.0000	1.0000	0.0000	1.0000	0.0000
4	0.7907	0.2093	0.8086	0.1914	0.8160	0.1840	0.8235	0.1765	0.8372	0.1628
5	0.3311	0.6689	0.3305	0.6695	0.2934	0.7066	0.3308	0.6692	0.2611	0.7389
6	0.0000	1.0000	0.0001	0.9999	0.0001	0.9999	0.0001	0.9999	0.0001	0.9999
7	0.0000	1.0000	0.0000	1.0000	0.0000	1.0000	0.0000	1.0000	0.0000	1.0000
8	0.0003	0.9997	0.0003	0.9997	0.0003	0.9997	0.0003	0.9997	0.0003	0.9997
	Data configuration 2)									
cluster	1	2	1	2	1	2	1	2	1	2
1	0.9999	0.0001	0.9999	0.0001	0.9999	0.0001	0.9999	0.0001	0.9999	0.0001
2	0.9999	0.0001	0.9999	0.0001	0.9999	0.0001	0.9999	0.0001	0.9999	0.0001
3	1.0000	0.0000	1.0000	0.0000	1.0000	0.0000	1.0000	0.0000	1.0000	0.0000
4	0.7407	0.2593	0.7654	0.2346	0.7715	0.2285	0.7860	0.2140	0.7976	0.2024
5	0.3889	0.6111	0.3848	0.6152	0.3457	0.6543	0.3824	0.6176	0.3083	0.6917
6	0.0000	1.0000	0.0001	0.9999	0.0001	0.9999	0.0001	0.9999	0.0001	0.9999
7	0.0000	1.0000	0.0000	1.0000	0.0000	1.0000	0.0000	1.0000	0.0000	1.0000
8	0.0003	0.9997	0.0003	0.9997	0.0003	0.9997	0.0003	0.9997	0.0004	0.9996
	Data configuration 3)									
cluster	1	2	1	2	1	2	1	2	1	2
1	0.9999	0.0001	0.9999	0.0001	0.9999	0.0001	0.9999	0.0001	0.9999	0.0001
2	0.9999	0.0001	0.9999	0.0001	0.9999	0.0001	0.9999	0.0001	0.9999	0.0001
3	1.0000	0.0000	1.0000	0.0000	1.0000	0.0000	1.0000	0.0000	1.0000	0.0000
4	0.6844	0.3156	0.7654	0.2346	0.7715	0.2285	0.7860	0.2140	0.7976	0.2024
5	0.4500	0.5500	0.3848	0.6152	0.3457	0.6543	0.3824	0.6176	0.3083	0.6917
6	0.0000	1.0000	0.0001	0.9999	0.0001	0.9999	0.0001	0.9999	0.0001	0.9999
7	0.0000	1.0000	0.0000	1.0000	0.0000	1.0000	0.0000	1.0000	0.0000	1.0000
8	0.0003	0.9997	0.0003	0.9997	0.0003	0.9997	0.0003	0.9997	0.0004	0.9996
	Data configuration 4)									
cluster	1	2	1	2	1	2	1	2	1	2
1	0.9999	0.0001	0.9999	0.0001	0.9999	0.0001	0.9999	0.0001	0.9999	0.0001
2	0.9999	0.0001	0.9999	0.0001	0.9999	0.0001	0.9999	0.0001	0.9999	0.0001
3	1.0000	0.0000	1.0000	0.0000	1.0000	0.0000	1.0000	0.0000	1.0000	0.0000
4	0.6271	0.3729	0.6853	0.3147	0.6689	0.3311	0.7168	0.2832	0.7051	0.2949
5	0.4874	0.5126	0.5256	0.4744	0.4603	0.5397	0.5169	0.4831	0.4138	0.5862
6	0.0000	1.0000	0.0000	1.0000	0.0001	0.9999	0.0000	1.0000	0.0001	0.9999
7	0.0000	1.0000	0.0000	1.0000	0.0000	1.0000	0.0000	1.0000	0.0000	1.0000
8	0.0003	0.9997	0.0001	0.9999	0.0004	0.9996	0.0001	0.9999	0.0004	0.9996

Note: Medoids' membership degrees are in bold.

Table A.8: Membership degrees for simulation study 1, according to different combinations of β_1 and β_2 and data configurations

Data configuration	(β_1, β_2)				
	(0, 0)	(4, 0)	(0, 4)	(8, 0)	0, 8
1)	0.82	0.82	0.81	0.81	0.80
2)	0.82	0.82	0.81	0.81	0.80
3)	0.84	0.82	0.81	0.81	0.80
4)	0.90	0.89	0.83	0.89	0.80

Table A.9: Fuzzy Silhouette index values for simulation study 1 according to different setting of the parameters β_1, β_2 (column wise) and to data configuration (row wise)

(β_1, β_2)	(8, 0)				(12, 0)				(16, 0)				(20, 0)				(0, 20)			
	1	2	3	4	1	2	3	4	1	2	3	4	1	2	3	4	1	2	3	4
cluster	Data configuration 1																			
1	0.9989	0.0005	0.0001	0.0005	0.9989	0.0005	0.0001	0.0005	0.9989	0.0005	0.0001	0.0005	0.9989	0.0005	0.0001	0.0005	0.9989	0.0005	0.0001	0.0005
2	0.9990	0.0004	0.0001	0.0004	0.9990	0.0004	0.0001	0.0004	0.9990	0.0004	0.0001	0.0004	0.9990	0.0004	0.0001	0.0004	0.9990	0.0004	0.0001	0.0004
3	1.0000	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000
4	0.8544	0.0608	0.0195	0.0654	0.9448	0.0232	0.0069	0.0250	0.8311	0.0698	0.0244	0.0746	0.9521	0.0200	0.0064	0.0215	0.8128	0.0767	0.0289	0.0816
5	0.0543	0.8801	0.0428	0.0229	0.0195	0.9577	0.0151	0.0077	0.0633	0.8571	0.0509	0.0287	0.0169	0.9628	0.0133	0.0070	0.0703	0.8384	0.0575	0.0338
6	0.0001	0.9997	0.0001	0.0000	0.0001	0.9997	0.0001	0.0000	0.0001	0.9996	0.0002	0.0001	0.0001	0.9997	0.0001	0.0000	0.0001	0.9997	0.0001	0.0000
7	0.0000	1.0000	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000
8	0.0009	0.9980	0.0008	0.0002	0.0008	0.9981	0.0008	0.0002	0.0008	0.9983	0.0007	0.0002	0.0008	0.9984	0.0007	0.0002	0.0008	0.9981	0.0008	0.0003
9	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
10	0.0001	0.0004	0.9990	0.0004	0.0001	0.0004	0.9990	0.0004	0.0001	0.0003	0.9992	0.0004	0.0001	0.0003	0.9992	0.0004	0.0001	0.0003	0.9993	0.0003
11	0.0000	0.0001	0.9997	0.0002	0.0000	0.0001	0.9998	0.0001	0.0000	0.0001	0.9997	0.0002	0.0000	0.0001	0.9996	0.0002	0.0000	0.0001	0.9996	0.0002
12	0.0235	0.0689	0.8523	0.0753	0.0095	0.0298	0.9279	0.0828	0.0288	0.0258	0.9372	0.0282	0.0334	0.0836	0.7928	0.0902	0.0081	0.0226	0.9448	0.0245
13	0.0425	0.0149	0.0400	0.9426	0.0108	0.0035	0.0101	0.9755	0.0523	0.0200	0.0494	0.8783	0.0093	0.0032	0.0088	0.9787	0.0601	0.0247	0.0569	0.8583
14	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000	1.0000
15	0.0002	0.0000	0.0002	0.9996	0.0002	0.0000	0.0002	0.9996	0.0002	0.0001	0.0002	0.9996	0.0001	0.0000	0.0001	0.9997	0.0002	0.0001	0.0002	0.9995
16	0.0001	0.0000	0.0002	0.9997	0.0001	0.0000	0.0001	0.9997	0.0001	0.0000	0.0001	0.9997	0.0001	0.0000	0.0001	0.9998	0.0001	0.0000	0.0001	0.9996
cluster	Data configuration 2																			
1	0.9987	0.0006	0.0001	0.0006	0.9986	0.0006	0.0001	0.0006	0.9986	0.0007	0.0001	0.0006	0.9986	0.0007	0.0001	0.0006	0.9985	0.0007	0.0002	0.0007
2	0.9989	0.0005	0.0001	0.0005	0.9989	0.0005	0.0001	0.0005	0.9989	0.0004	0.0001	0.0004	0.9987	0.0006	0.0001	0.0004	0.9987	0.0006	0.0002	0.0006
3	1.0000	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000
4	0.7265	0.1104	0.0417	0.1214	0.8210	0.0729	0.0280	0.0801	0.7172	0.1130	0.0464	0.1234	0.8437	0.0632	0.0241	0.0690	0.7102	0.1148	0.0505	0.1245
5	0.1016	0.7662	0.0800	0.6522	0.0656	0.8520	0.0508	0.0316	0.1047	0.7557	0.0842	0.0574	0.0568	0.8095	0.0449	0.0288	0.1069	0.7438	0.0876	0.0618
6	0.0002	0.9996	0.0002	0.0001	0.0001	0.9997	0.0002	0.0000	0.0002	0.9996	0.0002	0.0001	0.0001	0.9997	0.0001	0.0000	0.0002	0.9995	0.0002	0.0001
7	0.0000	1.0000	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000
8	0.0010	0.9978	0.0009	0.0003	0.0010	0.9978	0.0009	0.0003	0.0010	0.9978	0.0009	0.0003	0.0010	0.9978	0.0009	0.0003	0.0008	0.9983	0.0007	0.0002
9	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000	1.0000	0.0000
10	0.0001	0.0005	0.9988	0.0005	0.0001	0.0004	0.9990	0.0005	0.0002	0.0006	0.9987	0.0006	0.0001	0.0004	0.9991	0.0004	0.0002	0.0006	0.9985	0.0006
11	0.0000	0.0001	0.9996	0.0002	0.0000	0.0001	0.9997	0.0002	0.0001	0.0002	0.9994	0.0003	0.0000	0.0001	0.9997	0.0002	0.0001	0.0002	0.9993	0.0004
12	0.0402	0.1227	0.6918	0.1353	0.0324	0.0866	0.7863	0.0947	0.0539	0.1250	0.6853	0.1358	0.0301	0.0755	0.8125	0.0819	0.0579	0.1257	0.6807	0.1338
13	0.0796	0.0342	0.0737	0.8125	0.0439	0.0177	0.0407	0.8977	0.0849	0.0394	0.0791	0.7967	0.0377	0.0161	0.0351	0.9111	0.0889	0.0440	0.0833	0.7839
14	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000	1.0000
15	0.0002	0.0001	0.0002	0.9995	0.0002	0.0000	0.0002	0.9996	0.0002	0.0001	0.0002	0.9995	0.0002	0.0000	0.0002	0.9996	0.0002	0.0000	0.0002	0.9994
16	0.0001	0.0000	0.0002	0.9996	0.0001	0.0000	0.0002	0.9997	0.0001	0.0000	0.0002	0.9995	0.0001	0.0000	0.0002	0.9995	0.0001	0.0000	0.0002	0.9995

Note: Metastable membership degrees are in bold.

Table A.10: Membership degrees for simulation study 2, according to different combinations of β_1 and β_2 , and to data configurations 1) and 2)

(β_1, β_2)	(8, 0)				(12, 0)				(16, 0)				(20, 0)				(24, 0)							
	1	2	3	4	1	2	3	4	1	2	3	4	1	2	3	4	1	2	3	4				
cluster	Data configuration 3																							
1	0.5570	0.1876	0.0923	0.1631	0.5778	0.1770	0.0900	0.1552	0.5900	0.1665	0.0875	0.1471	0.5990	0.1708	0.0971	0.1471	0.9919	0.0024	0.0034	0.0023	0.9986	0.0006	0.0002	0.0006
2	0.5161	0.1878	0.1016	0.1945	0.5358	0.1793	0.0995	0.1854	0.5560	0.1708	0.0971	0.1762	0.5560	0.1708	0.0971	0.1762	0.9919	0.0024	0.0034	0.0023	0.9986	0.0006	0.0002	0.0006
3	0.5846	0.1625	0.0834	0.1695	0.6061	0.1532	0.0813	0.1593	0.6277	0.1440	0.0789	0.1494	0.6277	0.1440	0.0789	0.1494	1.0000	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000
4	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	0.3319	0.0905	0.4797	0.0980	0.7216	0.1059	0.0571	0.1154
5	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	0.0792	0.3131	0.5479	0.0599	0.0088	0.7493	0.0821	0.0697
6	0.1833	0.5154	0.2025	0.0987	0.1753	0.5352	0.1927	0.0968	0.1671	0.5555	0.1828	0.0946	0.1671	0.5555	0.1828	0.0946	0.0015	0.9934	0.0046	0.0005	0.0002	0.9995	0.0002	0.0001
7	0.1676	0.5741	0.1738	0.0845	0.1381	0.5958	0.1636	0.0825	0.1486	0.6177	0.1535	0.0801	0.1486	0.6177	0.1535	0.0801	0.0000	1.0000	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000
8	0.1875	0.5276	0.1885	0.0963	0.1786	0.5473	0.1796	0.0944	0.1786	0.5473	0.1796	0.0944	0.1786	0.5473	0.1796	0.0944	0.0000	1.0000	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000
9	0.0905	0.1460	0.5856	0.1780	0.0876	0.1382	0.6076	0.1666	0.0845	0.1303	0.6297	0.1554	0.0845	0.1303	0.6297	0.1554	0.0172	0.9482	0.8570	0.0771	0.0000	0.0000	0.0000	0.0000
10	0.0923	0.1611	0.5827	0.1639	0.0894	0.1518	0.6043	0.1545	0.0882	0.1426	0.6262	0.1451	0.0882	0.1426	0.6262	0.1451	0.0580	0.8640	0.0600	0.0002	0.0006	0.9986	0.0006	0.0006
11	0.0963	0.1523	0.5648	0.1865	0.0934	0.1447	0.5808	0.1752	0.0902	0.1369	0.6089	0.1640	0.0902	0.1369	0.6089	0.1640	0.0519	0.8466	0.0835	0.0001	0.0002	0.9994	0.0002	0.0003
12	0.0000	0.0000	1.0000	1.0000	0.0000	0.0000	1.0000	1.0000	0.0000	0.0000	1.0000	1.0000	0.0000	0.0000	1.0000	1.0000	0.0000	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
13	0.0000	0.0000	1.0000	1.0000	0.0000	0.0000	1.0000	1.0000	0.0000	0.0000	1.0000	1.0000	0.0000	0.0000	1.0000	1.0000	0.0756	0.0506	0.5051	0.3687	0.0451	0.0682	0.8135	0.8135
14	0.1381	0.0710	0.1385	0.6524	0.1271	0.0680	0.1274	0.6774	0.1165	0.0647	0.1167	0.7021	0.1165	0.0647	0.1167	0.7021	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000	1.0000
15	0.1575	0.0867	0.1411	0.6147	0.1459	0.0830	0.1317	0.6394	0.1347	0.0791	0.1224	0.6639	0.1347	0.0791	0.1224	0.6639	0.0017	0.0005	0.0045	0.9933	0.0002	0.0001	0.0002	0.9995
16	0.1534	0.0854	0.1660	0.5952	0.1437	0.0824	0.1547	0.6191	0.1341	0.0791	0.1437	0.6431	0.1341	0.0791	0.1437	0.6431	0.0004	0.0004	0.0040	0.9942	0.0001	0.0002	0.0001	0.9996
cluster	Data configuration 3																							
1	0.3476	0.2443	0.1817	0.2264	0.3627	0.2375	0.1787	0.2210	0.3781	0.2308	0.1756	0.2155	0.3781	0.2308	0.1756	0.2155	0.3038	0.2240	0.1723	0.2069	0.3038	0.2240	0.1723	0.2069
2	0.3343	0.2382	0.1866	0.2408	0.3475	0.2331	0.1840	0.2354	0.3610	0.2279	0.1812	0.2289	0.3610	0.2279	0.1812	0.2289	0.3750	0.2225	0.1783	0.2243	0.3750	0.2225	0.1783	0.2243
3	0.3579	0.2368	0.1743	0.2310	0.3745	0.2298	0.1714	0.2244	0.3912	0.2228	0.1683	0.2178	0.3912	0.2228	0.1683	0.2178	0.4081	0.2158	0.1650	0.2111	0.4081	0.2158	0.1650	0.2111
4	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
5	0.0000	1.0000	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000
6	0.2361	0.3240	0.2578	0.1821	0.2312	0.3375	0.2515	0.1799	0.2261	0.3513	0.2451	0.1775	0.2261	0.3513	0.2451	0.1775	0.2209	0.3656	0.2387	0.1749	0.2209	0.3656	0.2387	0.1749
7	0.2321	0.3441	0.2478	0.1760	0.2256	0.3610	0.2401	0.1732	0.2256	0.3610	0.2401	0.1732	0.2192	0.3780	0.2326	0.1702	0.2192	0.3951	0.2251	0.1670	0.2192	0.3951	0.2251	0.1670
8	0.2382	0.3419	0.2366	0.1833	0.2327	0.3552	0.2315	0.1807	0.2271	0.3688	0.2262	0.1779	0.2271	0.3688	0.2262	0.1779	0.2215	0.3828	0.2307	0.1750	0.2215	0.3828	0.2307	0.1750
9	0.1862	0.2135	0.3628	0.2375	0.1825	0.2081	0.3790	0.2304	0.1786	0.2026	0.3955	0.2233	0.1786	0.2026	0.3955	0.2233	0.1746	0.1969	0.4123	0.2162	0.1746	0.1969	0.4123	0.2162
10	0.1886	0.2199	0.3613	0.2303	0.1848	0.2141	0.3771	0.2240	0.1809	0.2082	0.3933	0.2176	0.1809	0.2082	0.3933	0.2176	0.1768	0.2022	0.4099	0.2111	0.1768	0.2022	0.4099	0.2111
11	0.1916	0.2150	0.3528	0.2406	0.1879	0.2100	0.3683	0.2338	0.1841	0.2048	0.3841	0.2270	0.1841	0.2048	0.3841	0.2270	0.1800	0.1995	0.4003	0.2302	0.1800	0.1995	0.4003	0.2302
12	0.0000	1.0000	1.0000	1.0000	0.0000	1.0000	1.0000	1.0000	0.0000	1.0000	1.0000	1.0000	0.0000	1.0000	1.0000	1.0000	0.0000	1.0000	1.0000	1.0000	0.0000	1.0000	1.0000	1.0000
13	0.0000	0.0000	1.0000	1.0000	0.0000	0.0000	1.0000	1.0000	0.0000	0.0000	1.0000	1.0000	0.0000	0.0000	1.0000	1.0000	0.0000	0.0000	1.0000	1.0000	0.0000	0.0000	1.0000	1.0000
14	0.2177	0.1674	0.2181	0.3968	0.2097	0.1635	0.2100	0.4168	0.2017	0.1592	0.2019	0.4372	0.2017	0.1592	0.2019	0.4372	0.1936	0.1547	0.1937	0.4580	0.1936	0.1547	0.1937	0.4580
15	0.2268	0.1878	0.2082	0.3773	0.2192	0.1830	0.2022	0.3956	0.2115	0.1780	0.1961	0.4144	0.2115	0.1780	0.1961	0.4144	0.2038	0.1728	0.1897	0.4338	0.2038	0.1728	0.1897	0.4338
16	0.2230	0.1758	0.2276	0.3736	0.2165	0.1724	0.2206	0.3904	0.2109	0.1687	0.2136	0.4079	0.2109	0.1687	0.2136	0.4079	0.2030	0.1647	0.2063	0.4259	0.2030	0.1647	0.2063	0.4259

Note: Metadist's membership degrees are in bold.

Table A.11: Membership degrees for simulation study 2, according to different combinations of β_1 and β_2 , and to data configurations 3) and 4)

Data configuration	(β_1, β_2)							
	8, 0	(0, 8)	(12, 0)	(0, 12)	(16, 0)	(0, 16)	(20, 0)	(0, 20)
1)	0.90	0.89	0.90	0.89	0.90	0.89	0.90	0.89
2)	0.84	0.82	0.84	0.82	0.84	0.82	0.84	0.82
3)	0.56	0.60	0.57	0.57	0.58	0.58	0.84	0.75
4)	0.16	0.16	0.23	0.23	0.26	0.26	0.29	0.29

Table A.12: Fuzzy Silhouette index values for simulation study 2 according to different setting of the parameters β_1, β_2 (column wise) and to data configuration (row wise)