Proceedings 1st International Workshop on Advanced Analytics and Learning on Temporal Data
AALTD 2015

Fuzzy Clustering of Series Using Quantile Autocovariances

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Abstract. Unlike conventional clustering, fuzzy cluster analysis allows data elements to belong to more than one cluster by assigning membership degrees of each data to clusters. This work proposes a fuzzy C–medoids algorithm to cluster time series based on comparing their estimated quantile autocovariance functions. The behaviour of the proposed algorithm is studied on different simulated scenarios and its effectiveness is concluded by comparison with alternative approaches.

1 Introduction

In classical cluster analysis each datum is assigned to exactly one cluster, thus producing a "hard" partition of the data set into several disjoint subsets. This approach can be inadequate in the presence of data objects that are equally distant to two ore more clusters. Fuzzy cluster analysis allows gradual memberships of data objects to clusters, thus providing versatility to reflect the certainty with which each data is assigned to the different clusters. An interesting overview of present fuzzy clustering methods is provided by [3]. Interest in this approach has increased in recent years. Proof of this is the large amount of publications in this field (e.g. [6] and [5]).

In this paper, a fuzzy C–medoids algorithm to cluster time series using the quantile autocovariance functions is proposed. Motivation behind this approach is twofold. First, quantile autocovariances have shown a high capability to cluster time series generated from a broad range of dependence models [10]. On the other hand, the use of a fuzzy approach for clustering time series is justified in order to gain adaptivity for constructing the centroids and to obtain a better characterization of the temporal pattern of the series (see discussion in [7]). To illustrate the merits of the proposed algorithm, an extensive simulation study comparing our fuzzy approach with other fuzzy procedures has been carried out. Specifically, we have focused on the classification of heteroskedastic models, which are of great importance in many applications (e.g. to model many financial time series) and have received relatively little attention in the clustering literature.

2 A dissimilarity based on quantile autocovariances

Consider a set of p series $S = \left\{\boldsymbol{X}^{(1)}, \ldots, \boldsymbol{X}^{(p)}\right\}$, with $\boldsymbol{X}^{(j)} = (X_1^{(j)}, \ldots, X_T^{(j)})$ being a T-length partial realization from a real valued process $\{X_t^{(j)},\ t \in \mathbb{Z}\}$.

We wish to perform cluster analysis on S in such a way that series with similar generating processes are grouped together. To achieve this goal, we propose to measure dissimilarity between two series by comparing the estimators of their quantile autocovariance functions (QAF), which are formally defined below.

Let $X_1, \ldots, X_T$ an observed stretch of a strictly stationary process $\{X_t;\ t \in \mathbb{Z}\}$. Denote by F the marginal distribution of X_t and by $q_\tau = F^{-1}(\tau)$, $\tau \in [0,1]$, the corresponding quantile function. Fixed $l \in \mathbb{Z}$ and an arbitrary couple of quantile levels $(\tau, \tau') \in [0,1]^2$, consider the cross-covariance of the indicator functions $I(X_t \leq q_\tau)$ and $I(X_{t+l} \leq q_{\tau'})$ given by

$$\gamma_l(\tau, \tau') = \operatorname{cov}\left\{I(X_t \leq q_\tau), I(X_{t+l} \leq q_{\tau'})\right\} = \mathbb{P}(X_t \leq q_\tau, X_{t+l} \leq q_{\tau'}) - \tau\tau'. \tag{1}$$

Function $\gamma_l(\tau, \tau')$, with $(\tau, \tau') \in [0,1]^2$, is called *quantile autocovariance function of lag l*. Replacing in (1) the theoretical quantiles of the marginal distribution F, q_τ and $q_{\tau'}$, by the corresponding empirical quantiles based on $X_1, \ldots, X_T$, $\hat{q}_\tau$ and $\hat{q}_{\tau'}$, we obtain the estimated quantile autocovariance function given by

$$\hat{\gamma}_l(\tau, \tau') = \frac{1}{T-l} \sum_{t=1}^{T-l} I(X_t \leq \hat{q}_\tau)\, I(X_{t+l} \leq \hat{q}_{\tau'}) - \tau\tau'. \tag{2}$$

As the quantile autocovariances are able to account for high level dynamic features, a simple dissimilarity criterion between two series $X_t^{(1)}$ and $X_t^{(2)}$ consists in comparing their estimated quantile autocovariances on a common range of selected quantiles. Thus, for L prefixed lags, $l_1, \ldots, l_L$, and r quantile levels, $0 < \tau_1 < \ldots < \tau_r < 1$, we construct the vectors $\boldsymbol{\Gamma}^{(u)}$, $u = 1, 2$, given by

$$\boldsymbol{\Gamma}^{(u)} = \left(\boldsymbol{\Gamma}_{l_1}^{(u)}, \ldots, \boldsymbol{\Gamma}_{l_L}^{(u)}\right), \quad \text{with} \quad \boldsymbol{\Gamma}_{l_i}^{(u)} = \left(\hat{\gamma}_{l_i}^{(u)}(\tau_j, \tau_k);\ j, k = 1 \ldots, r\right), \tag{3}$$

for $i = 1, \ldots, L$, and $\hat{\gamma}$ given in (2). Then, the distance between $X_t^{(1)}$ and $X_t^{(2)}$ is defined as the squared Euclidean distance between their representations $\boldsymbol{\Gamma}^{(1)}$ and $\boldsymbol{\Gamma}^{(2)}$, i.e.

$$d_{QAF}\left(X_t^{(1)}, X_t^{(2)}\right) = ||\boldsymbol{\Gamma}^{(1)} - \boldsymbol{\Gamma}^{(2)}||_2^2 \tag{4}$$

Computing d_{QAF} for all pairs of series in S allows us to set a pairwise dissimilarity matrix, which can be taken as starting point of a conventional hierarchical clustering algorithm. Alternatively, a partitioning clustering, such as the k-means algorithm, can be performed averaging the $\boldsymbol{\Gamma}$ representations to determine the centroids. Then, d_{QAF} is also used to calculate the distances between series and centroids involved in the iterative refinement of the cluster solution.

3 Fuzzy clustering based on quantile autocovariances

Time series are dynamic objects and therefore different temporal patterns may be necessary to characterize the serial behaviour in different periods of time. In other words, the series are not distributed accurately within a given number of clusters, but they can belong to two or even more clusters. This problem can be adequately treated using a fuzzy clustering procedure, which associates a fuzzy label vector to each element stating its memberships to the set of clusters. In this section we propose a fuzzy C-medoids clustering algorithm for time series by plugging the QAF-dissimilarity introduced in Section 2.

Let $S = \left\{\boldsymbol{X}^{(1)}, \ldots, \boldsymbol{X}^{(p)}\right\}$ be a set of p time series and $\boldsymbol{\Gamma} = \left\{\boldsymbol{\Gamma}^{(1)}, \ldots, \boldsymbol{\Gamma}^{(p)}\right\}$ a set of quantile autocovariances selected to perform clustering. The fuzzy C-medoids clustering finds the subset of $\boldsymbol{\Gamma}$, $\tilde{\boldsymbol{\Gamma}} = \left\{\tilde{\boldsymbol{\Gamma}}^{(1)}, \ldots, \tilde{\boldsymbol{\Gamma}}^{(C)}\right\}$, and the $p \times C$ matrix of fuzzy coefficients $\Omega = (u_{i,c})$ that lead to solve the minimization problem:

$$\min_{\tilde{\Gamma}, \Omega} \sum_{i=1}^{p} \sum_{c=1}^{C} u_{ic}^{m} \left\| \boldsymbol{\Gamma}^{(i)} - \boldsymbol{\Gamma}^{(c)} \right\|_2^2, \text{ subject to } \sum_{c=1}^{C} u_{ic} = 1 \text{ and } u_{ic} \geq 0. \quad (5)$$

Each $u_{ic} \in [0,1]$ represents the membership degree of the i-th series to the c-th cluster and the parameter $m > 1$ controls the fuzziness of the partition. As the value of m increases, the boundaries between clusters become softer and therefore the classification is fuzzier. If $m = 1$, the hard version of the clustering procedure is obtained, i.e. $u_{ic} \in \{0,1\}$, that leads to a classical K-means partition of S. The constraints $\sum_{c=1}^{C} u_{ic} = 1$ and $u_{ic} \geq 0$ ensure that no cluster is empty and that all series are included in the cluster partition.

The objective function (5) cannot be minimized directly, and an iterative algorithm that alternately optimizes the membership degrees and the medoids must be used. The update formula for the membership degrees is given by

$$u_{ic} = \left[\sum_{c'=1}^{C} \left(\frac{\left\| \boldsymbol{\Gamma}^{(i)} - \boldsymbol{\Gamma}^{(c)} \right\|_2^2}{\left\| \boldsymbol{\Gamma}^{(i)} - \boldsymbol{\Gamma}^{(c')} \right\|_2^2} \right)^{\frac{1}{m-1}} \right]^{-1}, \quad \text{for } i = 1, \ldots, p. \quad (6)$$

Then, the QAF-based fuzzy C–medoids clustering algorithm is implemented as follows.

i. Pick an initial set of medoids $\widetilde{\boldsymbol{\Gamma}} = \left\{\widetilde{\boldsymbol{\Gamma}}^{(1)}, \ldots, \widetilde{\boldsymbol{\Gamma}}^{(C)}\right\}$ and the fuzzifier m.
ii. Set $\widetilde{\boldsymbol{\Gamma}}_{\text{OLD}} = \widetilde{\boldsymbol{\Gamma}}$.
iii. Compute u_{ic} using (6).
iv. Update the medoids, let's say $\widehat{\boldsymbol{\Gamma}} = \left\{\widehat{\boldsymbol{\Gamma}}^{(1)}, \ldots, \widehat{\boldsymbol{\Gamma}}^{(C)}\right\}$, by minimizing the objective function with the new u_{ic}. Denote by

$$q = \text{argmin}_{1 \leq i' < p} \sum_{i''=1}^{p} u_{i''c}^{m} \left\| \boldsymbol{\Gamma}^{(i'')} - \boldsymbol{\Gamma}^{(i')} \right\|_2^2$$

If the value of q is lower than the one obtained with $\widetilde{\boldsymbol{\Gamma}}$, then $\widetilde{\boldsymbol{\Gamma}} = \widehat{\boldsymbol{\Gamma}}$.
v. If $\widetilde{\boldsymbol{\Gamma}}_{\text{OLD}} = \widetilde{\boldsymbol{\Gamma}}$ or a maximum number of iterations is achieved then end algorithm. Otherwise, return to step ii.

The total number of clusters C has to be preset. For this task classical indexes such as silhouette width or Krazanowski-Lai index can be used.

4 Simulation Study

The proposed fuzzy algorithm was tested against two other fuzzy clustering algorithms via simulation. In particular, the classification of heteroskedastic time series was considered by simulating two different scenarios formed by (i) GARCH(1,1) models and (ii) different structures of conditional heteroskedasticity. The selected generating models at each case are detailed below.

- **Scenario 1:** Consider $X_t = \mu_t + a_t$, with $\mu_t \sim$ AR(1) and $a_t = \sigma_t \epsilon_t$, $\epsilon_t \sim \mathcal{N}(0,1)$. Then, the following GARCH(1,1) structures for the varying conditional variance are considered:

  M1: $\sigma_t^2 = 0.1 + 0.01 a_{t-1}^2 + 0.9 \sigma_{t-1}^2$ M3: $\sigma_t^2 = 0.1 + 0.1 a_{t-1}^2 + 0.1 \sigma_{t-1}^2$
  M2: $\sigma_t^2 = 0.1 + 0.9 a_{t-1}^2 + 0.01 \sigma_{t-1}^2$ M4: $\sigma_t^2 = 0.1 + 0.4 a_{t-1}^2 + 0.5 \sigma_{t-1}^2$

- **Scenario 2:** Consider $X_t = \mu_t + a_t$, with $\mu_t \sim$ MA(1) and $a_t = \sigma_t \epsilon_t$, $\epsilon_t \sim \mathcal{N}(0,1)$. Then, the following ARCH(1), GARCH(1,1), GJR-GARCH and EGARCH structures are considered for the varying conditional variance:

  M1: $\sigma_t^2 = 0.1 + 0.8 a_{t-1}^2$
  M2: $\sigma_t^2 = 0.1 + 0.1 a_{t-1}^2 + 0.8 \sigma_{t-1}^2$
  M3: $\sigma_t^2 = 0.1 + (0.25 + 0.3 \mathrm{N}_{t-1}) a_{t-1}^2 + 0.5 \sigma_{t-1}^2$; $N_{t-1} = \mathrm{I}(a_{t-1} < 0)$
  M4: $\ln(\sigma_t^2) = 0.1 + \epsilon_{t-1} + 0.3 \left[|\epsilon_{t-1}| - \mathbb{E}(|\epsilon_{t-1}|) \right] + 0.4 \ln(\sigma_{t-1}^2)$

In all cases ϵ_t consisted of independent zero-mean Gaussian variables with unit variance. For each scenario, five series of length $T = 200$ were generated from each model over $N = 100$ trials.

Two fuzzy clustering algorithms specifically designed to deal with GARCH models were used and compared with our proposal. Both algorithms rely on different dissimilarity measures constructed using the AR representation of a GARCH(p,q) process given by

$$\sigma_t^2 = \gamma + \sum_{i=1}^{p} \alpha_i a_{t-i}^2 + \sum_{j=1}^{q} \beta_j \sigma_{t-j}^2 \tag{7}$$

with $\gamma > 0$, $0 \leq \alpha_i < 1$ and $0 \leq \beta_j < 1$, for $i = 1, \ldots, p$ and $j = 1, \ldots, q$, and $\left(\sum_{i=1}^{p} \alpha_i + \sum_{j=1}^{q} \beta_j\right) < 1$. Then, the dissimilarities are defined as follows.

1. Dissimilarity based on the autoregressive representation of the GARCH models [12, 11]. Given $\boldsymbol{X}^{(k)}$ and $\boldsymbol{X}^{(k')}$ in S, we define

   $$d_{AR}^2(\boldsymbol{X}^{(k)}, \boldsymbol{X}^{(k')}) = \sum_{r=1}^{R} \left(\widehat{\pi}_{rk} - \widehat{\pi}_{rk'}\right)^2,$$

   with $\widehat{\pi}_{rz}$ an estimator of the r-th coefficient $\pi_r = (\alpha_r + \beta_r) + \sum_{j=1}^{\min(q,r)} \beta_j \pi_{r-j}$, for the series z, $z = k, k'$. Parameter R determines the maximum number of autoregressive coefficients π_r. A GARCH–based fuzzy C-medoids clustering is proposed in [4] by considering the optimization problem:

$$\min_{\hat{\Pi},\Omega} \sum_{i=1}^{p} \sum_{c=1}^{C} u_{ic}^{m} \sum_{r=1}^{R} \left(\widehat{\pi}_{ri} - \widehat{\pi}_{rc}\right)^2, \text{ subject to } \sum_{c=1}^{C} u_{ic} = 1 \text{ and } u_{ic} \geq 0. \quad (8)$$

2. GARCH-based distance measure [1] given by

$$d_{\mathrm{GARCH}}(\boldsymbol{X}^{(k)}, \boldsymbol{X}^{(k')}) = \left(\boldsymbol{L_k} - \boldsymbol{L_{k'}}\right)' \left(\boldsymbol{V_k} + \boldsymbol{V_{k'}}\right)^{-1} \left(\boldsymbol{L_k} - \boldsymbol{L_{k'}}\right) \quad (9)$$

with $\boldsymbol{L_j} = \left(\widehat{\boldsymbol{\alpha}}_{\boldsymbol{j}}, \widehat{\boldsymbol{\beta}}_{\boldsymbol{j}}\right)$ the vector of estimated parameters and $\boldsymbol{V_j}$ the estimated covariance matrix for $\boldsymbol{L_j}$, for $j = k, k'$. An alternative GARCH-based fuzzy C-medoids clustering is proposed in [4] by minimizing:

$$\sum_{i=1}^{p} \sum_{c=1}^{C} u_{ic}^{m} \left[\left(\boldsymbol{L_i} - \boldsymbol{L_c}\right)' \left(\boldsymbol{V_i} + \boldsymbol{V_c}\right)^{-1} \left(\boldsymbol{L_i} - \boldsymbol{L_c}\right)\right], \quad (10)$$

subject to $\sum_{c=1}^{C} u_{ic} = 1$ and $u_{ic} \geq 0$.

The three fuzzy clustering algorithms were performed using a fuzziness parameter $m = 1.5$ on $N = 100$ trials for each scenario. At each trial, the quality of the clustering procedure was evaluated comparing the experimental cluster solution with the true cluster partition. Two different agreement measures were used, namely the Gavrilov index [8] and the adjusted Rand index [9]. The mean values and standard deviations of these indexes based on the 100 trials using both hard and fuzzy cluster analysis are provided in Table 1.

Table 1. Averages and standard deviations (in brackets) of two cluster similarity indexes obtained from 100 trials.

		Scenario 1		Scenario 2	
		Gavrilov	Adj. Rand	Gavrilov	Adj. Rand
Hard cluster	d_{AR}	0.859 (.109)	0.685 (.198)	0.712 (.146)	0.469 (.215)
	d_{GARCH}	0.574 (.059)	0.286 (.072)	0.504 (.078)	0.137 (.116)
	d_{QAF}	0.843 (.109)	0.726 (.152)	0.918 (.081)	0.825 (.135)
Fuzzy cluster	d_{AR}	0.541 (.056)	0.271 (.080)	0.486 (.076)	0.128 (.100)
	d_{GARCH}	0.553 (.088)	0.241 (.132)	0.535 (.076)	0.188 (.107)
	d_{QAF}	0.842 (.116)	0.704 (.181)	0.925 (.072)	0.833 (.125)

Results from Table 1 show that the metrics based on quantile autocovariances and on the AR representation led to the best scores in Scenario 1 when the hard cluster is carried out. When the fuzzy approaches were considered, the behaviour of the d_{AR} substantially worsened, while the very similar (even somewhat higher) results were obtained with d_{QAF}. The worst results were obtained with the GARCH-based dissimilarity both for the hard and the fuzzy versions.

The metric based on quantile autocovariances also obtained the best results in Scenario 2, with indexes of agreement above 0.8 and a slight improvement by using the fuzzy clustering. The GARCH-based metrics, d_{AR} and d_{GARCH} where strongly affected by the model misspecification and produced the worst results for both the hard and the fuzzy versions of the cluster analysis.

To assess the effect of the fuzziness parameter in the partitions the algorithm was implemented for several values of m. However this results were here omitted due to the limitation of space.

5 A case study

In this section, the proposed fuzzy C–medoids clustering algorithm is used to perform clustering on a set of series of electricity demand. Specifically, our database consists of hourly electricity demand in the Spanish market from 1st January 2011 to 31th December 2012. All data are sourced from the official website of Operador del Mercado Iberico de Energia[1]. Records corresponding to Saturdays and Sundays have been removed from the database because electricity demand is lower in the weekends. Thus we have 24 time series (one for each hour of the day) of length $T = 731$. Since all series are non–stationary in mean, the original series are transformed taking one regular difference.

Table 2 presents the membership degrees for the case with two and three clusters. The results obtained for the two–cluster partition formed by $C_1 = \{H24, H1, H2, H3, H4, H5, H6, H7\}$ and C_2 grouping the remaining series. The cluster C_1 corresponds with the hours of the day where the electricity demand is low, while the C_2 identifies the time of the day when the power consumption is greater. In the case of the three–cluster partition, the cluster C_1 is divided in two subclusters. One formed with the hours of the day with the lowest demand of electricity, and a second cluster with an intermediate electricity consumption.

6 Concluding remarks

In this paper, we focus on the classification of time series featuring a fuzzy clustering algorithm in the framework of a partitioning around medoids. A dissimilarity–based approach is considered. In particular, we propose a C–medoids fuzzy clustering algorithm using an innovative dissimilarity measure based on the quantile autocovariances (d_{QAF}).

The simulation study shows that the proposed dissimilarity produces satisfactory results by performing fuzzy cluster analysis. The proposed clustering algorithm was tested against two GARCH–based fuzzy clustering algorithm present in the literature in two different heteroskedastic scenarios. The fuzzy clustering algorithm based on d_{QAF} led to the best results. In fact, apart from d_{QAF}, none

[1] `http://http://www.omel.es/files/flash/ResultadosMercado.swf`

Table 2. Membership degrees obtained with QAF–based FCM with $m = 1.5$ considering 2 and 3 clusters.

	2 Clusters			3 Clusters			
	Membership degrees		Crisp	Membership degrees			Crisp
	C_1	C_2		C_1	C_2	C_3	
H1	0.63044	0.36956	1	1.00000	0.00000	0.00000	1
H2	1.00000	0.00000	1	0.99878	0.00098	0.00024	1
H3	0.98282	0.01718	1	0.99484	0.00395	0.00121	1
H4	0.94118	0.05882	1	0.99229	0.00574	0.00197	1
H5	1.00000	0.00000	1	0.92388	0.06811	0.00801	1
H6	0.99923	0.00077	1	0.30793	0.66185	0.03021	2
H7	0.98282	0.01718	1	0.00000	1.00000	0.00000	2
H8	0.00003	0.99997	2	0.05793	0.09475	0.84733	3
H9	0.00003	0.99997	2	0.00097	0.00294	0.99610	3
H10	0.00077	0.99923	2	0.00045	0.00149	0.99806	3
H11	0.00077	0.99923	2	0.00171	0.00507	0.99323	3
H12	0.00002	0.99998	2	0.00011	0.00049	0.99940	3
H13	0.00002	0.99998	2	0.00027	0.00178	0.99794	3
H14	0.00002	0.99998	2	0.00032	0.00107	0.99861	3
H15	0.00002	0.99998	2	0.00134	0.00940	0.98927	3
H16	0.00002	0.99998	2	0.00088	0.00636	0.99277	3
H17	0.00002	0.99998	2	0.00000	0.00000	1.00000	3
H18	0.00056	0.99944	2	0.00051	0.00498	0.99451	3
H19	0.00000	1.00000	2	0.00002	0.00014	0.99984	3
H20	0.00003	0.99997	2	0.00020	0.00135	0.99846	3
H21	0.00056	0.99944	2	0.00047	0.00384	0.99569	3
H22	0.01718	0.98282	2	0.00136	0.01488	0.98377	3
H23	0.00003	0.99997	2	0.01539	0.13091	0.85370	3
H24	0.99998	0.00002	1	0.00206	0.98054	0.01740	2

of the remaining examined dissimilarities shown acceptable results by clustering heteroskedastic processes, thus emphasizing the usefulness of d_{QAF} in this framework.

Note that a limitation of our procedure is that series are assumed to be strictly stationary and hence further research must be carried out. Although we have followed a dissimilarity-based approach, it is worthy to emphasize that model-based techniques can be also an interesting alternative. Likewise the fuzzy approach, the use of probabilistic models such as mixture models (see e.g. [2]) allows us to assign each datum to one single cluster although this assignment relies on a probabilistic approach since the mixing proportions are estimated from the data. Unlike the fuzzy approach, no fuzziness parameter is required by using mixture models, although the model selection problem must be solved in the latter case.

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