Journal of Machine Learning Research 17 (2016) 1-32

Submitted 7/13; Revised 12/14; Published 3/16

Consistent Algorithms for Clustering Time Series

Azadeh Khaleghi

A.KHALEGHI@LANCASTER.CO.UK

Department of Mathematics & Statistics Lancaster University, Lancaster, LA1 4YF, UK

Daniil Ryabko

DANIIL@RYABKO.NET

INRIA Lille 40, avenue de Halley 59650 Villeneuve d'Ascq, France

Jérémie Mary Philippe Preux JEREMIE.MARY@INRIA.FR PHILIPPE.PREUX@INRIA.FR

Université de Lille/CRIStAL (UMR CNRS) 40, avenue de Halley 59650 Villeneuve d'Ascq, France

Editor: Gábor Lugosi

Abstract

The problem of clustering is considered for the case where every point is a time series. The time series are either given in one batch (offline setting), or they are allowed to grow with time and new time series can be added along the way (online setting). We propose a natural notion of consistency for this problem, and show that there are simple, computationally efficient algorithms that are asymptotically consistent under extremely weak assumptions on the distributions that generate the data. The notion of consistency is as follows. A clustering algorithm is called consistent if it places two time series into the same cluster if and only if the distribution that generates them is the same. In the considered framework the time series are allowed to be highly dependent, and the dependence can have arbitrary form. If the number of clusters is known, the only assumption we make is that the (marginal) distribution of each time series is stationary ergodic. No parametric, memory or mixing assumptions are made. When the number of clusters is unknown, stronger assumptions are provably necessary, but it is still possible to devise nonparametric algorithms that are consistent under very general conditions. The theoretical findings of this work are illustrated with experiments on both synthetic and real data.

Keywords: clustering, time series, ergodicity, unsupervised learning

1. Introduction

Clustering is a widely studied problem in machine learning, and is key to many applications across different fields of science. The goal is to partition a given data set into a set of non-overlapping *clusters* in some natural way, thus hopefully revealing an underlying structure in the data. In particular, this problem for time series data is motivated by many research problems from a variety of disciplines, such as marketing and finance, biological and medical research, video/audio analysis, etc., with the common feature that the data are abundant while little is known about the nature of the processes that generate them.

The intuitively appealing problem of clustering is notoriously difficult to formalise. An intrinsic part of the problem is a similarity measure: the points in each cluster are supposed to be close to each other in some sense. While it is clear that the problem of finding the appropriate similarity measure is inseparable from the problem of achieving the clustering objectives, in the available formulations of the problem it is usually assumed that the similarity measure is given: it is either some fixed metric, or just a matrix of similarities between the points. Even with this simplification, it is still unclear how to define good clustering. Thus, Kleinberg (2002) presents a set of fairly natural properties that a good clustering function should have, and further demonstrate that there is no clustering function that satisfies these properties. A common approach is therefore to fix not only the similarity measure, but also some specific objective function — typically, along with the number of clusters — and to construct algorithms that maximise this objective. However, even this approach has some fundamental difficulties, albeit of a different, this time computational, nature: already in the case where the number of clusters is known, and the distance between the points is set to be the Euclidean distance, optimising some fairly natural objectives (such as k-means) turns out to be NP hard (Mahajan et al., 2009).

In this paper we consider a subset of the clustering problem, namely, clustering time series. That is, we consider the case where each data point is a sample drawn from some (unknown) time-series distribution. At first glance this does not appear to be a simplification (indeed, any data point can be considered as a time series of length 1). However, note that time series present a different dimension of asymptotic: with respect to their length, rather than with respect to the total number of points to be clustered. "Learning" along this dimension turns out to be easy to define, and allows for the construction of consistent algorithms under most general assumptions. Specifically, the assumption that each time series is generated by a stationary ergodic distribution is already sufficient to estimate any finite-dimensional characteristic of the distribution with arbitrary precision, provided the series is long enough. Thus, in contrast to the general clustering setup, in the time-series case it is possible to "learn" the distribution that generates each given data point. No assumptions on the dependence between time series are necessary for this. The assumption that a given time series is stationary ergodic is one of the most general assumptions used in statistics; in particular, it allows for arbitrary long-range serial dependence, and subsumes most of the nonparametric as well as modelling assumptions used in the literature on clustering time series, such as i.i.d., (hidden) Markov, or mixing time series.

This allows us to define the following clustering objective: group a pair of time series into the same cluster if and only if the distribution that generates them is the same.

Note that this intuitive objective is impossible to achieve outside the time-series framework. Even in the simplest case where the underlying distributions are Gaussian and the number of clusters is known, there is always a nontrivial likelihood for each point to be generated by any of the distributions. Thus, the best one can do is to estimate the parameters of the distributions, rather than to actually cluster the data points. The situation becomes hopeless in the nonparametric setting. In contrast, the fully nonparametric case is tractable for time-series data, both in offline and online scenarios, as explained in the next section.

1.1 Problem Setup

We consider two variants of the clustering problem in this setting: offline (batch) and online, defined as follows.

In the offline (batch) setting a finite number N of sequences $\mathbf{x}_1 = (X_1^1, \dots, X_{n_1}^1)$, $\dots, \mathbf{x}_N = (X_1^N, \dots, X_{n_N}^N)$ is given. Each sequence is generated by one of κ different unknown time-series distributions. The target clustering is the partitioning of $\mathbf{x}_1, \dots, \mathbf{x}_N$ into κ clusters, putting together those and only those sequences that were generated by the same time-series distribution. We call a batch clustering algorithm asymptotically consistent if, with probability 1, it stabilises on the target clustering in the limit as the lengths n_1, \dots, n_N of each of the N samples tend to infinity. The number κ of clusters may be either known or unknown. Note that the asymptotic is not with respect to the number of sequences, but with respect to the individual sequence lengths.

In the *online* setting we have a growing body of sequences of data. The number of sequences as well as the sequences themselves grow with time. The manner of this evolution can be arbitrary; we only require that the length of each individual sequence tend to infinity. Similarly to the batch setting, the joint distribution generating the data is unknown. At time step 1 initial segments of some of the first sequences are available to the learner. At each subsequent time step, new data are revealed, either as an extension of a previously observed sequence, or as a new sequence. Thus, at each time step t a total of N(t) sequences $\mathbf{x}_1, \ldots, \mathbf{x}_{N(t)}$ are to be clustered, where each sequence \mathbf{x}_i is of length $n_i(t) \in \mathbb{N}$ for i = 1..N(t). The total number of observed sequences N(t) as well as the individual sequence lengths $n_i(t)$ grow with time. In the online setting, a clustering algorithm is called asymptotically consistent, if almost surely for each fixed batch of sequences $\mathbf{x}_1, \ldots, \mathbf{x}_N$, the clustering restricted to this sequences coincides with the target clustering from some time on.

At first glance it may seem that one can use the offline algorithm in the online setting by simply applying it to the entire data observed at every time step. However, this naive approach does not result in a consistent algorithm. The main challenge in the online setting can be identified with what we regard as "bad" sequences: sequences for which sufficient information has not yet been collected, and thus cannot be distinguished based on the process distributions that generate them. In this setting, using a batch algorithm at every time step results in not only mis-clustering such "bad" sequences, but also in clustering incorrectly those for which sufficient data are already available. That is, such "bad" sequences can render the entire batch clustering useless, leading the algorithm to incorrectly cluster even the "good" sequences. Since new sequences may arrive in an uncontrollable (even data-dependent, adversarial) fashion, any batch algorithm will fail in this scenario.

1.2 Results

The first result of this work is a formal definition of the problem of time-series clustering which is rather intuitive, and at the same time allows for the construction of efficient algorithms that are provably consistent under the most general assumptions. The second result is the construction of such algorithms.

More specifically, we propose clustering algorithms that, as we further show, are strongly asymptotically consistent, provided that the number κ of clusters is known, and the process

distribution generating each sequence is stationary ergodic. No restrictions are placed on the dependence between the sequences: this dependence may be arbitrary (and can be thought of as adversarial). This consistency result is established in each of the two settings (offline and online) introduced above.

As follows from the theoretical impossibility results of Ryabko (2010c) that are discussed further in Section 1.4, under the only assumption that the distributions generating the sequences are stationary ergodic, it is impossible to find the correct number of clusters κ , that is, the total number of different time-series distributions that generate the data. Moreover, non-asymptotic results (finite-time bounds on the probability of error) are also provably impossible to obtain in this setting, since this is already the case for the problem of estimating the probability of any finite-time event (Shields, 1996).

Finding the number κ of clusters, as well as obtaining non-asymptotic performance guarantees, is possible under additional conditions on the distributions. In particular, we show that if κ is unknown, it is possible to construct consistent algorithms provided that the distributions are mixing and bounds on the mixing rates are available.

However, the main focus of this paper remains on the general framework where no additional assumptions on the unknown process distributions are made (other than that they are stationary ergodic). As such, the main theoretical and experimental results concern the case of known κ .

Finally, we show that our methods can be implemented efficiently: they are at most quadratic in each of their arguments, and are linear (up to log terms) in some formulations. To test the empirical performance of our algorithms we evaluated them on both synthetic and real data. To reflect the generality of the suggested framework in the experimental setup, we had our synthetic data generated by stationary ergodic process distributions that do not belong to any "simpler" class of distributions, and in particular cannot be modelled as hidden Markov processes with countable sets of states. In the batch setting, the error rates of both methods go to zero with sequence length. In the online setting with new samples arriving at every time step, the error rate of the offline algorithm remains consistently high, whereas that of the online algorithm converges to zero. This demonstrates that, unlike the offline algorithm, the online algorithm is robust to "bad" sequences. To demonstrate the applicability of our work to real-world scenarios, we chose the problem of clustering motion-capture sequences of human locomotion. This application area has also been studied in the works (Li and Prakash, 2011) and (Jebara et al., 2007) that (to the best of our knowledge) constitute the state-of-the-art performance¹ on the data sets they consider, and against which we compare the performance of our methods. We obtained consistently better performance on the data sets involving motion that can be considered ergodic (walking, running), and competitive performance on those involving non-ergodic motions (single jumps).

^{1.} After this paper had been accepted for publication and entered the production stage, the work (Tschannen and Bolcskei, 2015) appeared, which uses the data set of Li and Prakash (2011) and reports a better performance on it as compared to both our algorithm and that of Li and Prakash (2011).

1.3 Methodology and Algorithms

A crucial point of any clustering method is the similarity measure. Since the objective in our formulation is to cluster time series based on the distributions that generate them, the similarity measure must reflect the difference between the underlying distributions. As we aim to make as few assumptions as possible on the distributions that generate the data, and since we make no assumptions on the nature of differences between the distributions, the distance should take into account all possible differences between time-series distributions. Moreover, it should be possible to construct estimates of this distance that are consistent for arbitrary stationary ergodic distributions.

It turns out that a suitable distance for this purpose is the so-called distributional distance. The distributional distance $d(\rho_1, \rho_2)$ between a pair of process distributions ρ_1, ρ_2 is defined (Gray, 1988) as $\sum_{j\in\mathbb{N}} w_j |\rho_1(B_j) - \rho_2(B_j)|$ where, w_j are positive summable real weights, e.g. $w_i = 1/j(j+1)$, and B_i range over a countable field that generates the σ algebra of the underlying probability space. For example, consider finite-alphabet processes with the binary alphabet $\mathcal{X} = \{0,1\}$. In this case B_j , $j \in \mathbb{N}$ would range over the set $\mathcal{X}^* = \bigcup_{m \in \mathbb{N}} \mathcal{X}^m$; that is, over all tuples $0, 1, 00, 01, 10, 11, 000, 001, \ldots$; therefore, the distributional distance in this case is the weighted sum of the differences of the probability values (calculated with respect to ρ_1 and ρ_2) of all possible tuples. In this case, the distributional distance metrises the topology of weak convergence. In this work we consider real-valued processes so that the sets B_i range over a suitable sequence of intervals, all pairs of such intervals, triples, and so on (see the formal definitions in Section 2). Although this distance involves infinite summations, we show that its empirical approximations can be easily calculated. Asymptotically consistent estimates of this distance can be obtained by replacing unknown probabilities with the corresponding frequencies (Ryabko and Ryabko, 2010); these estimators have proved useful in various statistical problems concerning ergodic processes (Ryabko and Ryabko, 2010; Ryabko, 2012; Khaleghi and Ryabko, 2012).

Armed with an estimator of the distributional distance, it is relatively easy to construct a consistent clustering algorithm for the batch setting. In particular, we show that the following algorithm is asymptotically consistent. First, a set of κ cluster centres are chosen by κ farthest point initialisation (using an empirical estimate of the distributional distance). This means that the first sequence is assigned as the first cluster centre. Iterating over $2..\kappa$, at every iteration a sequence is sought which has the largest minimum distance from the already chosen cluster centres. Next, the remaining sequences are assigned to the closest clusters.

The online algorithm is based on a weighted combination of several clusterings, each obtained by running the offline procedure on different portions of data. The partitions are combined with weights that depend on the batch size and on an appropriate performance measure for each individual partition. The performance measure of each clustering is the minimum inter-cluster distance.

1.4 Related Work

Some probabilistic formulations of the time-series clustering problem can be considered related to ours. Perhaps the closest is in terms of mixture models (Bach and Jordan, 2004; Biernacki et al., 2000; Kumar et al., 2002; Smyth, 1997; Zhong and Ghosh, 2003):

it is assumed that the data are generated by a mixture of κ different distributions that have a particular known form (such as Gaussian, Hidden Markov models, or graphical models). Thus, each of the N samples is independently generated according to one of these κ distributions (with some fixed probability). Since the model of the data is specified quite well, one can use likelihood-based distances (and then, for example, the k-means algorithm), or Bayesian inference, to cluster the data. Another typical objective is to estimate the parameters of the distributions in the mixture (e.g., Gaussians), rather than actually clustering the data points. Clearly, the main difference between this setting and ours is in that we do not assume any known model for the data; we do not even require independence between the samples.

Taking a different perspective, the problem of clustering in our formulations generalises two classical problems in mathematical statistics, namely, homogeneity testing (or the twosample problem) and process classification (or the three-sample problem). In the two-sample problem, given two sequences $\mathbf{x}_1 = (X_1^1, \dots, X_{n_1}^1)$ and $\mathbf{x}_2 = (X_1^2, \dots, X_{n_2}^2)$ it is required to test whether they are generated by the same or by different process distributions. This corresponds to the special case of clustering only N=2 data points where the number κ of clusters is unknown: it can be either 1 or 2. In the three-sample problem, three sequences $\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3$ are given, and it is known that \mathbf{x}_1 and \mathbf{x}_2 are generated by different distributions, while \mathbf{x}_3 is generated either by the same distribution as \mathbf{x}_1 or by the same distribution as \mathbf{x}_2 . It is required to find which one is the case. This can be seen as clustering N=3 data points, with the number of clusters known: $\kappa = 2$. The classical approach is, of course, to consider Gaussian i.i.d. samples, but general nonparametric solutions exist not only for i.i.d. data (Lehmann, 1986), but also for Markov chains (Gutman, 1989), as well as under certain conditions on the mixing rates of the processes. Observe that the two-sample problem is more difficult to solve than the three-sample problem, since the number κ of clusters is unknown in the former while it is given in the latter. Indeed, as shown by Ryabko (2010c), in general for stationary ergodic (binary-valued) processes there is no solution for the twosample problem, even in the weakest asymptotic sense. A solution to the three-sample problem for (real-valued) stationary ergodic processes was given by (Ryabko and Ryabko, 2010); it is based on estimating the distributional distance.

More generally, the area of nonparametric statistical analysis of stationary ergodic time series to which the main results of this paper belong, is full of both positive and negative results, some of which are related to the problem of clustering in our formulation. Among these we can mention change point problems (Carlstein and Lele, 1994; Khaleghi and Ryabko, 2012, 2014) hypothesis testing (Ryabko, 2012, 2014; Morvai and Weiss, 2005) and prediction (Ryabko, 1988; Morvai and Weiss, 2012).

1.5 Organization

The remainder of the paper is organised as follows. We start by introducing notation and definitions in Section 2. In Section 3 we define the considered clustering protocol. Our main theoretical results are given in Section 4, where we present our methods, prove their consistency, and discuss some extensions (Section 4.4). Section 5 is devoted to computational considerations. In Section 6 we provide some experimental evaluations on both synthetic and real data. Finally, in Section 7 we provide some concluding remarks and open questions.

2. Preliminaries

Let \mathcal{X} be a measurable space (the domain); in this work we let $\mathcal{X} = \mathbb{R}$ but extensions to more general spaces are straightforward. For a sequence X_1, \ldots, X_n we use the abbreviation $X_{1..n}$. Consider the Borel σ -algebra \mathcal{B} on \mathcal{X}^{∞} generated by the cylinders $\{B \times \mathcal{X}^{\infty} : B \in B^{m,l}, m, l \in \mathbb{N}\}$ where, the sets $B^{m,l}, m, l \in \mathbb{N}$ are obtained via the partitioning of \mathcal{X}^m into cubes of dimension m and volume 2^{-ml} (starting at the origin). Let also $B^m := \bigcup_{l \in \mathbb{N}} B^{m,l}$. We may choose any other means to generate the Borel σ -algebra \mathcal{B} on \mathcal{X} , but we need to fix a specific choice for computational reasons. Process distributions are probability measures on the space $(\mathcal{X}^{\infty}, \mathcal{B})$. Similarly, one can define distributions over the space $((\mathcal{X}^{\infty})^{\infty}, \mathcal{B}_2)$ of infinite matrices with the Borel σ -algebra \mathcal{B}_2 generated by the cylinders $\{(\mathcal{X}^{\infty})^k \times (B \times \mathcal{X}^{\infty}) \times (\mathcal{X}^{\infty})^{\infty} : B \in B^{m,l}, k, m, l \in \{0\} \cup \mathbb{N}\}$. For $\mathbf{x} = X_{1..n} \in \mathcal{X}^n$ and $B \in B^m$ let $\nu(\mathbf{x}, B)$ denote the frequency with which \mathbf{x} falls in B, i.e.

$$\nu(\mathbf{x}, B) := \frac{\mathbb{I}\{n \ge m\}}{n - m + 1} \sum_{i=1}^{n - m + 1} \mathbb{I}\{X_{i..i + m - 1} \in B\}$$
 (1)

A process ρ is stationary if for any $i, j \in 1...n$ and $B \in \mathcal{B}$, we have

$$\rho(X_{1..i} \in B) = \rho(X_{i..i+i-1} \in B).$$

A stationary process ρ is called *ergodic* if for all $B \in \mathcal{B}$ with probability 1 we have

$$\lim_{n \to \infty} \nu(X_{1..n}, B) = \rho(B).$$

By virtue of the ergodic theorem (e.g., Billingsley, 1961), this definition can be shown to be equivalent to the standard definition of stationary ergodic processes (every shift-invariant set has measure 0 or 1; see, e.g., Gray, 1988).

Definition 1 (Distributional Distance) The distributional distance between a pair of process distributions ρ_1, ρ_2 is defined as follows (Gray, 1988):

$$d(\rho_1, \rho_2) = \sum_{m,l=1}^{\infty} w_m w_l \sum_{B \in B^{m,l}} |\rho_1(B) - \rho_2(B)|,$$

where we set $w_j := 1/j(j+1)$, but any summable sequence of positive weights may be used.

In words, this involves partitioning the sets \mathcal{X}^m , $m \in \mathbb{N}$ into cubes of decreasing volume (indexed by l) and then taking a sum over the absolute differences in probabilities of all of the cubes in these partitions. The differences in probabilities are weighted: smaller weights are given to larger m and finer partitions.

Remark 2 The distributional distance is more generally defined as

$$d'(\rho_1, \rho_2) := \sum_{i \in \mathbb{N}} w_i |\rho_1(A_i) - \rho_2(A_i)|$$

where A_i ranges over a countable field that generates the σ -algebra of the underlying probability space (Gray, 1988). Definition 1 above is more suitable for implementing and testing

algorithms, while the consistency results of this paper hold for either. Note also that the choice of sets B_i may result in a different topology on the space of time-series distributions. The particular choice we made results in the usual topology of weak convergence (Billingsley, 1999).

We use the following empirical estimates of the distributional distance.

Definition 3 (Empirical estimates of d) Define the empirical estimate of the distributional distance between a sequence $\mathbf{x} = X_{1..n} \in \mathcal{X}^n, n \in \mathbb{N}$ and a process distribution ρ as

$$\hat{d}(\mathbf{x}, \rho) := \sum_{m=1}^{m_n} \sum_{l=1}^{l_n} w_m w_l \sum_{B \in B^{m,l}} |\nu(\mathbf{x}, B) - \rho(B)|,$$
 (2)

and that between a pair of sequences $\mathbf{x}_i \in \mathcal{X}^{n_i}$ $n_i \in \mathbb{N}$, i = 1, 2 as

$$\hat{d}(\mathbf{x}_1, \mathbf{x}_2) := \sum_{m=1}^{m_n} \sum_{l=1}^{l_n} w_m w_l \sum_{B \in B^{m,l}} |\nu(\mathbf{x}_1, B) - \nu(\mathbf{x}_2, B)|,$$
(3)

where m_n and l_n are any sequences that go to infinity with n, and $(w_j)_{j\in\mathbb{N}}$ are as in Definition 1.

Remark 4 (constants m_n, l_n) The sequences of constants $m_n, l_n (n \in \mathbb{N})$ in the definition of \hat{d} are intended to introduce some computational flexibility in the estimate: while already the choice $m_n, l_n \equiv \infty$ is computationally feasible, other choices give better computational complexity without sacrificing the quality of the estimate; see Section 5. For the asymptotic consistency results this choice is irrelevant. Thus, in the proofs we tacitly assume $m_n, l_n \equiv \infty$; extension to the general case is straightforward.

Lemma 5 (\hat{d} is asymptotically consistent: Ryabko and Ryabko, 2010) For every pair of sequences $\mathbf{x}_1 \in \mathcal{X}^{n_1}$ and $\mathbf{x}_2 \in \mathcal{X}^{n_2}$ with joint distribution ρ whose marginals $\rho_i, i = 1, 2$ are stationary ergodic we have

$$\lim_{n_1, n_2 \to \infty} \hat{d}(\mathbf{x}_1, \mathbf{x}_2) = d(\rho_1, \rho_2), \ \rho - a.s., \ and$$
 (4)

$$\lim_{n_i \to \infty} \hat{d}(\mathbf{x}_i, \rho_j) = d(\rho_i, \rho_j), \ i, j \in 1, 2, \ \rho - a.s.$$
 (5)

The proof of this lemma can be found in the work (Ryabko and Ryabko, 2010); since it is important for further development but rather short and simple, we reproduce it here.

Proof The idea of the proof is simple: for each set $B \in \mathcal{B}$, the frequency with which the sample \mathbf{x}_i , i = 1, 2 falls into B converges to the probability $\rho_i(B)$, i = 1, 2. When the sample sizes grow, there will be more and more sets $B \in \mathcal{B}$ whose frequencies have already converged to the corresponding probabilities, so that the cumulative weight of those sets whose frequencies have not converged yet will tend to 0.

Fix $\varepsilon > 0$. We can find an index J such that

$$\sum_{m,l=J}^{\infty} w_m w_l \le \varepsilon/3.$$

Moreover, for each $m, l \in 1...J$ we can find a finite subset $S^{m,l}$ of $B^{m,l}$ such that

$$\rho_i(S^{m,l}) \ge 1 - \frac{\varepsilon}{6Jw_m w_l}.$$

There exists some N (which depends on the realization $X_1^i, \ldots, X_{n_i}^i, i = 1, 2$) such that for all $n_i \geq N$, i = 1, 2 we have,

$$\sup_{B \in S^{m,l}} |\nu(\mathbf{x}_i, B) - \rho_i(B)| \le \frac{\varepsilon \rho_i(B)}{6J w_m w_l}, \ i = 1, 2.$$

$$(6)$$

For all $n_i \geq N$, i = 1, 2 we have

$$\begin{aligned} |\hat{d}(\mathbf{x}_{1}, \mathbf{x}_{2}) - d(\rho_{1}, \rho_{2})| &= \left| \sum_{m,l=1}^{\infty} w_{m} w_{l} \sum_{B \in B^{m,l}} \left(|\nu(\mathbf{x}_{1}, B) - \nu(\mathbf{x}_{2}, B)| - |\rho_{1}(B) - \rho_{2}(B)| \right) \right| \\ &\leq \sum_{m,l=1}^{\infty} w_{m} w_{l} \sum_{B \in B^{m,l}} |\nu(\mathbf{x}_{1}, B) - \rho_{1}(B)| + |\nu(\mathbf{x}_{2}, B) - \rho_{2}(B)| \\ &\leq \sum_{m,l=1}^{J} w_{m} w_{l} \sum_{B \in S^{m,l}} \left(|\nu(\mathbf{x}_{1}, B) - \rho_{1}(B)| + |\nu(\mathbf{x}_{2}, B) - \rho_{2}(B)| \right) + 2\varepsilon/3 \\ &\leq \sum_{m,l=1}^{J} w_{m} w_{l} \sum_{B \in S^{m,l}} \frac{\rho_{1}(B)\varepsilon}{6Jw_{m}w_{l}} + \frac{\rho_{2}(B)\varepsilon}{6Jw_{m}w_{l}} + 2\varepsilon/3 \leq \varepsilon, \end{aligned}$$

which proves (4). The statement (5) can be proven analogously.

Remark 6 The triangle inequality holds for the distributional distance $d(\cdot, \cdot)$ and its empirical estimates $\hat{d}(\cdot, \cdot)$ so that for all distributions ρ_i , i = 1..3 and all sequences $\mathbf{x}_i \in \mathcal{X}^{n_i}$ $n_i \in \mathbb{N}$, i = 1..3 we have

$$d(\rho_1, \rho_2) \leq d(\rho_1, \rho_3) + d(\rho_2, \rho_3),$$

$$\hat{d}(\mathbf{x}_1, \mathbf{x}_2) \leq \hat{d}(\mathbf{x}_1, \mathbf{x}_3) + \hat{d}(\mathbf{x}_2, \mathbf{x}_3),$$

$$\hat{d}(\mathbf{x}_1, \rho_1) \leq \hat{d}(\mathbf{x}_1, \rho_2) + d(\rho_1, \rho_2).$$

3. Clustering Settings: Offline and Online

We start with a common general probabilistic setup for both settings (offline and online), which we use to formulate each of the two settings separately.

Consider the matrix $\mathbf{X} \in (\mathcal{X}^{\infty})^{\infty}$ of random variables

$$\mathbf{X} := \begin{bmatrix} X_1^1 & X_2^1 & X_3^1 & \dots \\ X_1^2 & X_2^2 & \dots & \dots \\ \vdots & \vdots & \ddots & \vdots \end{bmatrix} \in (\mathcal{X}^{\infty})^{\infty}$$
 (7)

generated by some probability distribution P on $((\mathcal{X}^{\infty})^{\infty}, \mathcal{B}_2)$. Assume that the marginal distribution of P on each row of \mathbf{X} is one of κ unknown stationary ergodic process distributions $\rho_1, \rho_2, \ldots, \rho_{\kappa}$. Thus, the matrix \mathbf{X} corresponds to infinitely many one-way infinite sequences, each of which is generated by a stationary ergodic distribution. Aside from this assumption, we do not make any further assumptions on the distribution P that generates \mathbf{X} . This means that the rows of \mathbf{X} (corresponding to different time-series samples) are allowed to be dependent, and the dependence can be arbitrary; one can even think of the dependence between samples as adversarial. For notational convenience we assume that the distributions $\rho_k, k = 1..\kappa$ are ordered based on the order of appearance of their first rows (samples) in \mathbf{X} .

Among the various ways the rows of X may be partitioned into κ disjoint subsets, the most natural partitioning in this formulation is to group together those and only those rows for which the marginal distribution is the same. More precisely, we define the ground-truth partitioning of X as follows.

Definition 7 (Ground-truth G) Let

$$\mathcal{G} = \{\mathcal{G}_1, \dots, \mathcal{G}_\kappa\}$$

be a partitioning of \mathbb{N} into κ disjoint subsets \mathcal{G}_k , $k = 1..\kappa$, such that the marginal distribution of \mathbf{x}_i , $i \in \mathbb{N}$ is ρ_k for some $k \in 1..\kappa$ if and only if $i \in \mathcal{G}_k$. We call \mathcal{G} the ground-truth clustering. We also introduce the notation $\mathcal{G}|_N$ for the restriction of \mathcal{G} to the first N sequences:

$$\mathcal{G}|_{N} := \{\mathcal{G}_{k} \cap \{1..N\} : k = 1..\kappa\}.$$

3.1 Offline Setting

The problem is formulated as follows. We are given a finite set $S := \{\mathbf{x}_1, \dots, \mathbf{x}_N\}$ of N samples, for some fixed $N \in \mathbb{N}$. Each sample is generated by one of κ unknown stationary ergodic process distributions $\rho_1, \dots, \rho_{\kappa}$. More specifically, the set S is obtained from \mathbf{X} as follows. Some (arbitrary) lengths $n_i \in \mathbb{N}$, $i \in 1..N$ are fixed, and \mathbf{x}_i for each i = 1..N is defined as $\mathbf{x}_i := X_{1..n_i}^i$.

A clustering function f takes a finite set $S := \{\mathbf{x}_1, \dots, \mathbf{x}_N\}$ of samples and an optional parameter κ (the number of target clusters) to produce a partition $f(S, \kappa) := \{C_1, \dots, C_\kappa\}$ of the index set $\{1..N\}$. The goal is to partition $\{1..N\}$ so as to recover the ground-truth clustering $\mathcal{G}|_N$. For consistency of notation, in the offline setting we identify \mathcal{G} with $\mathcal{G}|_N$. We call a clustering algorithm asymptotically consistent if it achieves this goal for long enough sequences \mathbf{x}_i , i = 1..N in S:

Definition 8 (Consistency: offline setting) A clustering function f is consistent for a set of sequences S if $f(S,\kappa) = \mathcal{G}$. Moreover, denoting $n := \min\{n_1,\ldots,n_N\}$, f is called strongly asymptotically consistent in the offline sense if with probability 1 from some n on it is consistent on the set S: $P(\exists n' \forall n > n' f(S,\kappa) = \mathcal{G}) = 1$. It is weakly asymptotically consistent if $\lim_{n\to\infty} P(f(S,\kappa) = \mathcal{G}) = 1$.

Note that the notion of consistency above is asymptotic with respect to the minimum sample length n, and not with respect to the number N of samples.

When considering the offline setting with a known number of clusters κ we assume that N is such that $\{1..N\} \cap \mathcal{G}_k \neq \emptyset$ for every $k = 1..\kappa$ (that is, all κ clusters are represented); otherwise we could just take a smaller κ .

3.2 Online Setting

The online problem is formulated as follows. Consider the infinite matrix **X** given by (7). At every time step $t \in \mathbb{N}$, a part S(t) of **X** is observed corresponding to the first $N(t) \in \mathbb{N}$ rows of **X**, each of length $n_i(t), i \in 1...N(t)$, i.e.

$$S(t) = {\mathbf{x}_1^t, \cdots \mathbf{x}_{N(t)}^t}$$
 where $\mathbf{x}_i^t := X_{1..n_i(t)}^i$.

This setting is depicted in Figure 1. We assume that the number of samples, as well as the individual sample-lengths grow with time. That is, the length $n_i(t)$ of each sequence \mathbf{x}_i is nondecreasing and grows to infinity (as a function of time t). The number of sequences N(t) also grows to infinity. Aside from these assumptions, the functions N(t) and $n_i(t)$ are completely arbitrary.

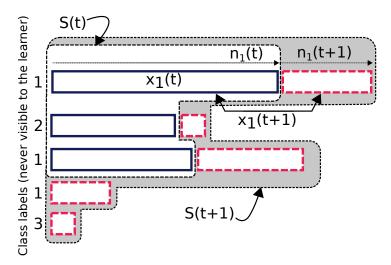


Figure 1: Online Protocol: solid rectangles correspond to sequences available at time t, dashed rectangles correspond to segments arrived at time t + 1.

An online clustering function is strongly asymptotically consistent if, with probability 1, for each $N \in \mathbb{N}$ from some time on the first N sequences are clustered correctly (with respect to the ground-truth given by Definition 7).

Definition 9 (Consistency: online setting) A clustering function is strongly (weakly) asymptotically consistent in the online sense, if for every $N \in \mathbb{N}$ the clustering $f(S(t), \kappa)|_N$ is strongly (weakly) asymptotically consistent in the offline sense, where $f(S(t), \kappa)|_N$ is the clustering $f(S(t), \kappa)$ restricted to the first N sequences:

$$f(S(t), \kappa)|_{N} := \{f(S(t), \kappa) \cap \{1..N\}, k = 1..\kappa\}.$$

Remark 10 Note that even if the *eventual* number κ of different time-series distributions producing the sequences (that is, the number of clusters in the ground-truth clustering \mathcal{G}) is known, the number of observed distributions at each individual time step is unknown. That is, it is possible that at a given time t we have $|\mathcal{G}|_{N(t)}| < \kappa$.

Known and unknown κ . As mentioned in the introduction, in the general framework described above, consistent clustering (for both the offline and the online problems) with unknown number of clusters is impossible. This follows from the impossibility result of Ryabko (2010c) that states that when we have only two (binary-valued) samples generated (independently) by two stationary ergodic distributions, it is impossible to decide whether they have been generated by the same or by different distributions, even in the sense of weak asymptotic consistency. (This holds even if the distributions come from a smaller class: the set of all B-processes.) Therefore, if the number of clusters is unknown, we are bound to make stronger assumptions. Since our main interest in this paper is to develop consistent clustering algorithms under the general framework described above, for the most part of this paper we assume that the correct number κ of clusters is known. However, in Section 4.3 we also show that under certain mixing conditions on the process distributions that generate the data, it is possible to have consistent algorithms in the case of unknown κ as well.

4. Clustering Algorithms and their Consistency

In this section we present our clustering methods for both the offline and the online settings. The main results, presented in Sections 4.1 (offline) and 4.2 (online), concern the case where the number of clusters κ is known. In Section 4.3 we show that, given the mixing rates of the process distributions that generate the data, it is possible to find the correct number of clusters κ and thus obtain consistent algorithms for the case of unknown κ as well. Finally, Section 4.4 considers some extensions of the proposed settings.

4.1 Offline Setting

Given that we have asymptotically consistent estimates d of the distributional distance d, it is relatively simple to construct asymptotically consistent clustering algorithms for the offline setting. This follows from the fact that, since $\hat{d}(\cdot,\cdot)$ converges to $d(\cdot,\cdot)$, for large enough sequence lengths n the points $\mathbf{x}_1, \ldots, \mathbf{x}_N$ have the so-called strict separation property: the points within each target cluster are closer to each other than to points in any other cluster (on strict separation in clustering see, for example, Balcan et al., 2008). This makes many simple algorithms, such as single or average linkage, or the k-means algorithm with certain initialisations, provably consistent.

We present below one specific algorithm that we show to be asymptotically consistent in the general framework introduced. What makes this simple algorithm interesting is that it requires only κN distance calculations (that is, much less than is needed to calculate the distance between each two sequences). In short, Algorithm 1 initialises the clusters using farthest-point initialisation, and then assigns each remaining point to the nearest cluster. More precisely, the sample \mathbf{x}_1 is assigned as the first cluster centre. Then a sample is found that is farthest away from \mathbf{x}_1 in the empirical distributional distance \hat{d} and is assigned as

the second cluster centre. For each $k=2..\kappa$ the $k^{\rm th}$ cluster centre is sought as the sequence with the largest minimum distance from the already assigned cluster centres for 1..k-1. (This initialisation was proposed for use with k-means clustering by Katsavounidis et al., 1994.) By the last iteration we have κ cluster centres. Next, the remaining samples are each assigned to the closest cluster.

```
Algorithm 1 Offline clustering
```

```
1: INPUT: sequences S := \{\mathbf{x}_1, \cdots, \mathbf{x}_N\}, Number \kappa of clusters

2: Initialize \kappa-farthest points as cluster-centres:

3: c_1 \leftarrow 1

4: C_1 \leftarrow \{c_1\}

5: for k = 2..\kappa do

6: c_k \leftarrow \underset{i=1..N}{\operatorname{argmax}} \underset{j=1..k-1}{\operatorname{min}} \hat{d}(\mathbf{x}_i, \mathbf{x}_{c_j}), where ties are broken arbitrarily

7: C_k \leftarrow \{c_k\}

8: end for

9: Assign the remaining points to closest centres:

10: for i = 1..N do

11: k \leftarrow \underset{j=1..N}{\operatorname{argmin}}_{j \in \bigcup_{k=1}^{\kappa} C_k} \hat{d}(\mathbf{x}_i, \mathbf{x}_j)

12: C_k \leftarrow C_k \cup \{i\}

13: end for

14: OUTPUT: clusters C_1, C_2, \cdots, C_{\kappa}
```

Theorem 11 Algorithm 1 is strongly asymptotically consistent (in the offline sense of Definition 8), provided that the correct number κ of clusters is known, and the marginal distribution of each sequence \mathbf{x}_i , i = 1..N is stationary ergodic.

Proof To prove the consistency statement we use Lemma 5 to show that if the samples in S are long enough, the samples that are generated by the same process distribution are closer to each other than to the rest of the samples. Therefore, the samples chosen as cluster centres are each generated by a different process distribution, and since the algorithm assigns the rest of the samples to the closest clusters, the statement follows. More formally, let n denote the shortest sample length in S:

$$n_{\min} := \min_{i \in 1..N} n_i.$$

Denote by δ the minimum nonzero distance between the process distributions:

$$\delta := \min_{k \neq k' \in 1..\kappa} \hat{d}(\rho_k, \rho_{k'}).$$

Fix $\varepsilon \in (0, \delta/4)$. Since there are a finite number N of samples, by Lemma 5 for all large enough n_{\min} we have

$$\sup_{\substack{k \in 1...\kappa \\ i \in \mathcal{G}_k \cap \{1..N\}}} \hat{d}(\mathbf{x}_i, \rho_k) \le \varepsilon. \tag{8}$$

where \mathcal{G}_k , $k = 1..\kappa$ denote the ground-truth partitions given by Definition 7. By (8) and applying the triangle inequality we obtain

$$\sup_{\substack{k \in 1..\kappa \\ i,j \in \mathcal{G}_k \cap \{1..N\}}} \hat{d}(\mathbf{x}_i, \mathbf{x}_j) \le 2\varepsilon. \tag{9}$$

Thus, for all large enough n_{\min} we have

$$\inf_{\substack{i \in \mathcal{G}_k \cap \{1..N\} \\ j \in \mathcal{G}_{k'} \cap \{1..N\} \\ k \neq k' \in 1..\kappa}} \hat{d}(\mathbf{x}_i, \mathbf{x}_j) \ge \inf_{\substack{i \in \mathcal{G}_k \cap \{1..N\} \\ j \in \mathcal{G}_{k'} \cap \{1..N\} \\ k \neq k' \in 1..\kappa}} d(\rho_k, \rho_{k'}) - \hat{d}(\mathbf{x}_i, \rho_k) - \hat{d}(\mathbf{x}_j, \rho_{k'})$$

$$\ge \delta - 2\varepsilon$$
(10)

where the first inequality follows from the triangle inequality, and the second inequality follows from (8) and the definition of δ . In words, (9) and (10) mean that the samples in \mathcal{S} that are generated by the same process distribution are closer to each other than to the rest of the samples. Finally, for all n_{\min} large enough to have (9) and (10) we obtain

$$\max_{i=1..N} \min_{k=1..\kappa-1} \hat{d}(\mathbf{x}_i, \mathbf{x}_{c_k}) \geq \delta - 2\varepsilon > \delta/2$$

where as specified by Algorithm 1, $c_1 := 1$ and $c_k := \underset{i=1..N}{\operatorname{argmax}} \min_{j=1..k-1} \hat{d}(\mathbf{x}_i, \mathbf{x}_{c_j}), \ k = 2..\kappa$. Hence, the indices c_1, \ldots, c_{κ} will be chosen to index sequences generated by different process distributions. To derive the consistency statement, it remains to note that, by (9) and (10), each remaining sequence will be assigned to the cluster centre corresponding to the sequence generated by the same distribution.

4.2 Online Setting

The online version of the problem turns out to be more complicated than the offline one. The challenge is that, since new sequences arrive (potentially) at every time step, we can never rely on the distance estimates corresponding to all of the observed samples to be correct. Thus, as mentioned in the introduction, the main challenge can be identified with what we regard as "bad" sequences: recently-observed sequences, for which sufficient information has not yet been collected, and for which the estimates of the distance (with respect to any other sequence) are bound to be misleading. Thus, in particular, farthest-point initialisation would not work in this case. More generally, using any batch algorithm on all available data at every time step results in not only mis-clustering "bad" sequences, but also in clustering incorrectly those for which sufficient data are already available.

The solution, realised in Algorithm 2, is based on a weighted combination of several clusterings, each obtained by running the offline algorithm (Algorithm 1) on different portions of data. The clusterings are combined with weights that depend on the batch size and on the minimum inter-cluster distance. This last step of combining multiple clusterings with weights may be reminiscent of prediction with expert advice (see Cesa-Bianchi and Lugosi, 2006 for an overview), where experts are combined based on their past performance.

Algorithm 2 Online Clustering

```
1: INPUT: Number \kappa of target clusters
 2: for t = 1..\infty do
           Obtain new sequences S(t) = \{\mathbf{x}_1^t, \dots, \mathbf{x}_{N(t)}^t\}
 4:
           Initialize the normalization factor: \eta \leftarrow 0
           Initialize the final clusters: C_k(t) \leftarrow \emptyset, k = 1..\kappa
 5:
 6:
           Generate N(t) - \kappa + 1 candidate cluster centres:
           for j = \kappa .. N(t) do
 7:
                \{C_1^j,\ldots,C_\kappa^j\}\leftarrow \text{Alg1}(\{\mathbf{x}_1^t,\cdots,\mathbf{x}_i^t\},\kappa)
 8:
                \mu_k \leftarrow \min\{i \in C_k^j\}, k = 1..\kappa
                                                                              ▶ Set the smallest index as cluster centre.
 9:
                (c_1^j, \ldots, c_\kappa^j) \leftarrow \operatorname{sort}(\mu_1, \ldots, \mu_\kappa)
                                                                                   ▷ Sort the cluster centres increasingly.
10:
                \gamma_j \leftarrow \min_{k \neq k' \in 1..\kappa} \hat{d}(\mathbf{x}_{c_k^j}^t, \mathbf{x}_{c_{k'}^j}^t)
                                                                                               ▶ Calculate performance score.
11:
                w_i \leftarrow 1/j(j+1)
12:
                \eta \leftarrow \eta + w_i \gamma_i
13:
           end for
14:
           Assign points to clusters:
15:
           for i = 1..N(t) do
16:
                k \leftarrow \operatorname{argmin}_{k' \in 1..\kappa} \frac{1}{\eta} \sum_{j=1}^{N(t)} w_j \gamma_j \hat{d}(\mathbf{x}_i^t, \mathbf{x}_{c_{.,}^j}^t)
17:
                C_k(t) \leftarrow C_k(t) \cup \{i\}
18:
19:
           OUTPUT: \{C_1(t), \cdots, C_k(t)\}
20:
21: end for
```

However, the difference here is that the performance of each clustering cannot be measured directly.

More precisely, Algorithm 2 works as follows. Given a set S(t) of N(t) samples, the algorithm iterates over $j:=\kappa,\ldots,N(t)$ where at each iteration Algorithm 1 is used to cluster the first j sequences $\{\mathbf{x}_1^t,\ldots,\mathbf{x}_j^t\}$ into κ clusters. In each cluster the sequence with the smallest index is assigned as the candidate cluster centre. A performance score γ_j is calculated as the minimum distance \hat{d} between the κ candidate cluster centres obtained at iteration j. Thus, γ_j is an estimate of the minimum inter-cluster distance. At this point we have $N(t) - \kappa + 1$ sets of κ cluster centres $c_1^j,\ldots,c_\kappa^j,\ j=1..N(t)-\kappa+1$. Next, every sample $\mathbf{x}_i^t,\ i=1..N(t)$ is assigned to a cluster, according to the weighted combination of the distances between \mathbf{x}_i^t and the candidate cluster centres obtained at each iteration on j. More precisely, for each i=1..N(t) the sequence \mathbf{x}_i^t is assigned to the cluster κ , where κ is defined as

$$k := \operatorname{argmin}_{k=1..\kappa} \sum_{j=\kappa}^{N(t)} w_j \gamma_j \hat{d}(\mathbf{x}_i^t, \mathbf{x}_{c_k^j}^t).$$

Theorem 12 Algorithm 2 is strongly asymptotically consistent (in the online sense of Definition 9), provided the correct number of clusters κ is known, and the marginal distribution of each sequence \mathbf{x}_i , $i \in \mathbb{N}$ is stationary ergodic.

Before giving the proof of Theorem 12, we provide an intuitive explanation as to how Algorithm 2 works. First, consider the following simple candidate solution. Take some fixed (reference) portion of the samples, run the batch algorithm on it, and then simply assign every remaining sequence to the nearest cluster. Since the offline algorithm is asymptotically consistent, this procedure would be asymptotically consistent as well, but only if we knew that the selected reference of the sequences contains at least one sequence sampled from each and every one of the κ distributions. However, there is no way to find a fixed (not growing with time) portion of data that would be guaranteed to contain a representative of each cluster (that is, of each time-series distribution). Allowing such a reference set of sequences to grow with time would guarantee that eventually it contains representatives of all clusters, but it would break the consistency guarantee for the reference set; since the set grows, this formulation effectively returns us back to the original online clustering problem.

A key observation we make to circumvent this problem is the following. If, for some $j \in \{\kappa, \dots, N(t)\}$, each sample in the batch $\{\mathbf{x}_1^t, \dots, \mathbf{x}_j^t\}$ is generated by at most $\kappa - 1$ process distributions, any partitioning of this batch into κ sets results in a minimum intercluster distance γ_j that, as follows from the asymptotic consistency of \hat{d} , converges to 0. On the other hand, if the set of samples $\{\mathbf{x}_1^t, \dots, \mathbf{x}_j^t\}$ contains sequences generated by all κ process distributions, γ_j converges to a nonzero constant, namely, the minimum distance between the distinct process distributions $\rho_1, \dots, \rho_{\kappa}$. In the latter case from some time on the batch $\{\mathbf{x}_1^t, \dots, \mathbf{x}_j^t\}$ will be clustered correctly. Thus, instead of selecting one reference batch of sequences and constructing a set of clusters based on those, we consider all batches of sequences for $j = \kappa ... N(t)$, and combine them with weights. Two sets of weights are involved in this step: γ_j and w_j , where

- 1. γ_j is used to penalise for small inter-cluster distance, cancelling the clustering results produced based on sets of sequences generated by less than κ distributions;
- 2. w_j is used to give precedence to chronologically earlier clusterings, protecting the clustering decisions from the presence of the (potentially "bad") newly formed sequences, whose corresponding distance estimates may still be far from accurate.

As time goes on, the batches in which not all clusters are represented will have their weight γ_j converge to 0, while the number of batches that have all clusters represented and are clustered correctly by the offline algorithm will go to infinity, and their total weight will approach 1. Note that, since we are combining different clusterings, it is important to use a consistent ordering of clusters, for otherwise we might sum up clusters generated by different distributions. Therefore, we always order the clusters with respect to the index of the first sequence in each cluster.

Proof [of Theorem 12] First, we show that for every $k \in 1..\kappa$ we have

$$\frac{1}{\eta} \sum_{j=1}^{N(t)} w_j \gamma_j^t \hat{d}(\mathbf{x}_{c_k^j}^t, \rho_k) \to 0 \text{ a.s.}$$

$$\tag{11}$$

Denote by δ the minimum nonzero distance between the process distributions:

$$\delta := \min_{k \neq k' \in 1..\kappa} \hat{d}(\rho_k, \rho_{k'}). \tag{12}$$

Fix $\varepsilon \in (0, \delta/4)$. We can find an index J such that $\sum_{j=J}^{\infty} w_j \leq \varepsilon$. Let $S(t)|_j = \{\mathbf{x}_1^t, \dots, \mathbf{x}_j^t\}$ denote the subset of S(t) consisting of the first j sequences for $j \in 1..N(t)$. For $k = 1..\kappa$ let

$$s_k := \min\{i \in \mathcal{G}_k \cap 1..N(t)\} \tag{13}$$

index the first sequence in S(t) that is generated by ρ_k where \mathcal{G}_k , $k = 1...\kappa$ are the ground-truth partitions given by Definition 7. Define

$$m := \max_{k \in 1, \kappa} s_k. \tag{14}$$

Recall that the sequence lengths $n_i(t)$ grow with time. Therefore, by Lemma 5 (consistency of \hat{d}) for every $j \in 1...J$ there exists some $T_1(j)$ such that for all $t \geq T_1(j)$ we have

$$\sup_{\substack{k \in 1...\kappa \\ i \in \mathcal{G}_k \cap \{1..j\}}} \hat{d}(\mathbf{x}_i^t, \rho_k) \le \varepsilon. \tag{15}$$

Moreover, by Theorem 11 for every $j \in m...J$ there exists some $T_2(j)$ such that $\text{Alg1}(S(t)|_j, \kappa)$ is consistent for all $t \geq T_2(j)$. Let

$$T := \max_{\substack{i=1,2\\j \in 1...J}} T_i(j).$$

Recall that, by definition (14) of m, $S(t)|_m$ contains samples from all κ distributions. Therefore, for all $t \geq T$ we have

$$\inf_{k \neq k' \in 1...\kappa} \hat{d}(\mathbf{x}_{c_k^m}^t, \mathbf{x}_{c_{k'}^m}^t) \ge \inf_{k \neq k' \in 1...\kappa} d(\rho_k, \rho_{k'}) - \sup_{k \neq k' \in 1...\kappa} (\hat{d}(\mathbf{x}_{c_k^m}^t, \rho_k) + \hat{d}(\mathbf{x}_{c_{k'}^m}^t, \rho_{k'}))$$

$$\ge \delta - 2\varepsilon \ge \delta/2, \tag{16}$$

where the first inequality follows from the triangle inequality and the second inequality follows from the consistency of $\mathrm{Alg1}(S(t)|_m,\kappa)$ for $t\geq T$, the definition of δ given by (12) and the assumption that $\varepsilon\in(0,\delta/4)$. Recall that (as specified in Algorithm 2) we have $\eta:=\sum_{j=1}^{N(t)}w_j\gamma_j^t$. Hence, by (16) for all $t\geq T$ we have

$$\eta \ge w_m \delta/2. \tag{17}$$

By (17) and noting that by definition, $\hat{d}(\cdot,\cdot) \leq 1$ for all $t \geq T$, for every $k \in 1...\kappa$ we obtain

$$\frac{1}{\eta} \sum_{j=1}^{N(t)} w_j \gamma_j^t \hat{d}(\mathbf{x}_{c_k^j}^t, \rho_k) \le \frac{1}{\eta} \sum_{j=1}^J w_j \gamma_j^t \hat{d}(\mathbf{x}_{c_k^j}^t, \rho_k) + \frac{2\varepsilon}{w_m \delta}.$$
 (18)

On the other hand, by the definition (14) of m, the sequences in $S(t)|_j$ for j=1..m-1 are generated by $at \ most \ \kappa-1$ out of the κ process distributions. Therefore, at every iteration on $j\in 1..m-1$ there exists at least one pair of distinct cluster centres that are generated by the same process distribution. Therefore, by (15) and (17), for all $t\geq T$ and every $k\in 1..\kappa$ we have,

$$\frac{1}{\eta} \sum_{j=1}^{m-1} w_j \gamma_j^t \hat{d}(\mathbf{x}_{c_k^j}^t, \rho_i) \le \frac{1}{\eta} \sum_{j=1}^{m-1} w_j \gamma_j^t \le \frac{2\varepsilon}{w_m \delta}.$$
 (19)

Noting that the clusters are ordered in the order of appearance of the distributions, we have $\mathbf{x}_{c_k^j}^t = \mathbf{x}_{s_k}^t$ for all j = m..J and $k = 1..\kappa$, where the index s_k is defined by (13). Therefore, by (15) for all $t \geq T$ and every $k = 1..\kappa$ we have

$$\frac{1}{\eta} \sum_{j=m}^{J} w_j \gamma_j^t \hat{d}(\mathbf{x}_{c_k^j}^t, \rho_k) = \frac{1}{\eta} \hat{d}(\mathbf{x}_{s_k}^t, \rho_k) \sum_{j=m}^{J} w_j \gamma_j^t \le \varepsilon.$$
 (20)

Combining (18), (19), and (20) we obtain

$$\frac{1}{\eta} \sum_{j=1}^{N(t)} w_j \gamma_j^t \hat{d}(\mathbf{x}_{c_k^j}^t, \rho_k) \le \varepsilon (1 + \frac{4}{w_m \delta}). \tag{21}$$

for all $k = 1..\kappa$ and all $t \ge T$, establishing (11).

To finish the proof of the consistency, consider an index $i \in \mathcal{G}_r$ for some $r \in 1..\kappa$. By Lemma 5, increasing T if necessary, for all $t \geq T$ we have

$$\sup_{\substack{k \in 1...\kappa \\ j \in \mathcal{G}_k \cap 1..N}} \hat{d}(\mathbf{x}_j^t, \rho_k) \le \varepsilon. \tag{22}$$

For all $t \geq T$ and all $k \neq r \in 1..\kappa$ we have,

$$\frac{1}{\eta} \sum_{j=1}^{N(t)} w_j \gamma_j^t \hat{d}(\mathbf{x}_i^t, \mathbf{x}_{c_k^j}^t) \ge \frac{1}{\eta} \sum_{j=1}^{N(t)} w_j \gamma_j^t \hat{d}(\mathbf{x}_i^t, \rho_k) - \frac{1}{\eta} \sum_{j=1}^{N(t)} w_j \gamma_j^t \hat{d}(\mathbf{x}_{c_k^j}^t, \rho_k)$$

$$\ge \frac{1}{\eta} \sum_{j=1}^{N(t)} w_j \gamma_j^t (\hat{d}(\rho_k, \rho_r) - \hat{d}(\mathbf{x}_i^t, \rho_r)) - \frac{1}{\eta} \sum_{j=1}^{N(t)} w_j \gamma_j^t \hat{d}(\mathbf{x}_{c_k^j}^t, \rho_k)$$

$$\ge \delta - 2\varepsilon (1 + \frac{2}{w_m \delta}), \tag{23}$$

where the first and second inequalities follow from the triangle inequality, and the last inequality follows from (22), (21) and the definition of δ . Since the choice of ε is arbitrary, from (22) and (23) we obtain

$$\underset{k \in 1...\kappa}{\operatorname{argmin}} \frac{1}{\eta} \sum_{j=1}^{N(t)} w_j \gamma_j^t \hat{d}(\mathbf{x}_i^t, \mathbf{x}_{c_k^j}^t) = r.$$
 (24)

It remains to note that for any fixed $N \in \mathbb{N}$ from some t on (24) holds for all i = 1..N, and the consistency statement follows.

4.3 Unknown Number κ of Clusters

So far we have shown that when κ is known in advance, consistent clustering is possible under the only assumption that the samples are generated by unknown stationary ergodic process distributions. However, as follows from the theoretical impossibility results

of Ryabko (2010c) discussed in Section 3, the correct number κ of clusters is not possible to be estimated with no further assumptions or additional constraints. One way to overcome this obstacle is to assume known rates of convergence of frequencies to the corresponding probabilities. Such rates are provided by assumptions on the mixing rates of the process distributions that generate the data.

Here we will show that under some assumptions on the mixing rates (and still without making any modelling or independence assumptions), consistent clustering is possible when the number of clusters is unknown.

The purpose of this section, however, is not to find the weakest assumptions under which consistent clustering (with κ unknown) is possible, nor is it to provide sharp bounds under the assumptions considered; our only purpose here is to demonstrate that asymptotic consistency is achievable in principle when the number of clusters is unknown, under some mild nonparametric assumptions on the time-series distributions. More refined analysis could yield sharper bounds under weaker assumptions, such as those in, for example, (Bosq, 1996; Rio, 1999; Doukhan, 1994; Doukhan et al., 2010).

We introduce mixing coefficients, mainly following Rio (1999) in formulations. Informally, mixing coefficients of a stochastic process measure how fast the process forgets about its past. Any one-way infinite stationary process X_1, X_2, \ldots can be extended backwards to make a two-way infinite process $\ldots, X_{-1}, X_0, X_1, \ldots$ with the same distribution. In the definition below we assume such an extension. Define the φ -mixing coefficients of a process μ as

$$\varphi_n(\mu) = \sup_{A \in \sigma(X_{-\infty..k}), B \in \sigma(X_{k+n..\infty}), \mu(A) \neq 0} |\mu(B|A) - \mu(B)|, \tag{25}$$

where $\sigma(...)$ stands for the σ -algebra generated by random variables in brackets. These coefficients are nonincreasing. Define also

$$\theta_n(\mu) := 2 + 8(\varphi_1(\mu) + \dots + \varphi_n(\mu)).$$

A process μ is called uniformly φ -mixing if $\varphi_n(\mu) \to 0$. Many important classes of processes satisfy mixing conditions. For example, a stationary irreducible aperiodic Hidden Markov process with finitely many states is uniformly φ -mixing with coefficients decreasing exponentially fast. Other probabilistic assumptions can be used to obtain bounds on the mixing coefficients, see, e.g., (Bradley, 2005) and references therein.

The method that we propose for clustering mixing time series in the offline setting, namely $Algorithm\ 3$, is very simple. Its inputs are: a set $S:=\{\mathbf{x}_1,\ldots,\mathbf{x}_N\}$ of samples each of length $n_i,\ i=1..N$, the threshold level $\delta\in(0,1)$ and the parameters $m,l\in\mathbb{N},\ B^{m,l,n}$. The algorithm assigns to the same cluster all samples which are at most δ -far from each other, as measured by \hat{d} with $m_n=m,l_n=l$ and the summation over $B^{m,l}$ restricted to $B^{m,l,n}$. The sets $B^{m,l,n}$ have to be chosen so that in asymptotic they cover the whole space, $\bigcup_{n\in\mathbb{N}}B^{m,l,n}=B^{m,l}$. For example, $B^{m,l,n}$ may consist of the first b_n cubes around the origin, where $b_n\to\infty$ is a parameter sequence. We do not give a pseudocode implementation of this algorithm, since it is rather clear.

The idea is that the threshold level $\delta = \delta_n$ is selected according to the smallest samplelength $n := \min_{i=1..N} n_i$ and the (known bounds on) mixing rates of the process ρ generating the samples (see Theorem 13). As we show in Theorem 13, if the distribution of the samples satisfies $\varphi_n(\rho) \leq \varphi_n \to 0$, where φ_n are known, then one can select (based on φ_n only) the parameters of Algorithm 3 in such a way that it is weakly asymptotically consistent. Moreover, a bound on the probability of error before asymptotic is provided.

Theorem 13 (Algorithm 3 is consistent for unknown κ) Fix sequences $m_n, l_n, b_n \in \mathbb{N}$, and let, for each $m, l \in \mathbb{N}$, $B^{m,l,n} \subset B^{m,l}$ be an increasing sequence of finite sets such that $\bigcup_{n \in \mathbb{N}} B^{m,l,n} = B^{m,l}$. Set $b_n := \max_{1 \le l_n, m \le m_n} |B^{m,l,n}|$ and $n := \min_{i=1..N} n_i$. Let also $\delta_n \in (0,1)$. Let $N \in \mathbb{N}$, and suppose that the samples $\mathbf{x}_1, \ldots, \mathbf{x}_N$ are generated in such a way that the (unknown marginal) distributions ρ_k , $k = 1..\kappa$ are stationary ergodic and satisfy $\varphi_n(\rho_k) \le \varphi_n$, for all $k = 1..\kappa$, $n \in \mathbb{N}$. Then there exist constants ε_ρ , δ_ρ and n_ρ that depend only on ρ_k , $k = 1..\kappa$, such that for all $\delta_n < \delta_\rho$ and $n > n_\rho$, Algorithm 3 satisfies

$$P(T \neq \mathcal{G}|_{N}) \le 2N(N+1)(m_{n}l_{n}b_{n}\gamma_{n/2}(\delta_{n}) + \gamma_{n/2}(\varepsilon_{\rho}))$$
(26)

where

$$\gamma_n(\varepsilon) := \sqrt{e} \exp(-n\varepsilon^2/\theta_n),$$

T is the partition output by the algorithm and $\mathcal{G}|_N$ is the ground-truth clustering. In particular, if $\varphi_n = o(1)$, then, selecting the parameters in such a way that $\delta_n = o(1)$, $m_n, l_n, b_n = o(n)$, $m_n, l_n \to \infty$, $\cup_{k \in \mathbb{N}} B^{m,l,k} = B^{m,l}$, $b_n^{m,l} \to \infty$, for all $m, l \in \mathbb{N}$, $\gamma_n(const) = o(1)$, and, finally, $m_n l_n b_n \gamma_n(\delta_n) = o(1)$, as is always possible, Algorithm 3 is weakly asymptotically consistent (with the number of clusters κ unknown).

Proof We use the following bound from (Rio, 1999, Corollary 2.1): for any zero-mean [-1,1]-valued random process $Y_1,Y_2,...$ with distribution P and every $n \in \mathbb{N}$ we have

$$P\left(\left|\sum_{i=1}^{n} Y_{i}\right| > n\varepsilon\right) \leq \gamma_{n}(\varepsilon). \tag{27}$$

For every j = 1..N, every m < n, $l \in \mathbb{N}$, and $B \in B^{m,l}$, define the [-1,1]-valued processes $\mathbf{Y}^j := Y_1^j, Y_2^j, \ldots$ as

$$Y_t^j := \mathbb{I}\{(X_t^j, \dots, X_{t+m-1}^j) \in B\} - \rho_k(X_{1,m}^j \in B),$$

where ρ_k is the marginal distribution of X^j (that is, k is such that $j \in \mathcal{G}_k$). It is easy to see that φ -mixing coefficients for this process satisfy $\varphi_n(\mathbf{Y}^j) \leq \varphi_{n-2m}$. Thus, from (27) we have

$$P(|\nu(X_{1..n_i}^j, B) - \rho_k(X_{1..m}^j \in B)| > \varepsilon/2) \le \gamma_{n-2m_n}(\varepsilon/2).$$
 (28)

Then for every $i, j \in \mathcal{G}_k \cap 1..N$ for some $k \in 1..\kappa$ (that is, \mathbf{x}_i and \mathbf{x}_j are in the same ground-truth cluster) we have

$$P(|\nu(X_{1..n_i}^i, B) - \nu(X_{1..n_i}^j, B)| > \varepsilon) \le 2\gamma_{n-2m_n}(\varepsilon/2).$$

Using the union bound, summing over m, l, and B, we obtain

$$P(\hat{d}(\mathbf{x}_i, \mathbf{x}_j) > \varepsilon) \le 2m_n l_n b_n \gamma_{n-2m_n}(\varepsilon/2). \tag{29}$$

Next, let $i \in \mathcal{G}_k \cap 1..N$ and $j \in \mathcal{G}_{k'} \cap 1..N$ for $k \neq k' \in 1..\kappa$ (i.e., $\mathbf{x}_i, \mathbf{x}_j$ are in two different target clusters). Then, for some $m_{i,j}, l_{i,j} \in \mathbb{N}$ there is $B_{i,j} \in B^{m_{i,j}, l_{i,j}}$ such that for some $\tau_{i,j} > 0$ we have

$$|\rho_k(X_{1..|B_{i,j}|}^i \in B_{i,j}) - \rho_{k'}(X_{1..|B_{i,j}|}^j \in B_{i,j})| > 2\tau_{i,j}.$$

Then for every $\varepsilon < \tau_{i,j}/2$ we have

$$P(|\nu(X_{1..n_i}^i, B_{i,j}) - \nu(X_{1..n_i}^j, B_{i,j})| < \varepsilon) \le 2\gamma_{n-2m_{i,j}}(\tau_{i,j}).$$
(30)

Moreover, for $\varepsilon < w_{m_{i,j}} w_{l_{i,j}} \tau_{i,j}/2$ we have

$$P(\hat{d}(\mathbf{x}_i, \mathbf{x}_j) < \varepsilon) \le 2\gamma_{n-2m_{i,j}}(\tau_{i,j}). \tag{31}$$

Define

$$\delta_{\rho} := \min_{\substack{k \neq k' \in 1..\kappa \\ i \in \mathcal{G}_k \cap 1..N \\ j \in \mathcal{G}_{k'} \cap 1..N}} w_{m_{i,j}} w_{l_{i,j}} \tau_{i,j}/2, \quad \varepsilon_{\rho} := \min_{\substack{k \neq k' \in 1..\kappa \\ i \in \mathcal{G}_k \cap 1..N \\ j \in \mathcal{G}_{k'} \cap 1..N}} \tau_{i,j}/2$$

$$n_{\rho} := 2 \max_{\substack{k \neq k' \in 1..\kappa \\ i \in \mathcal{G}_k \cap 1..N \\ j \in \mathcal{G}_{k'} \cap 1..N}} m_{i,j}.$$

Clearly, from this and (30), for every $\delta < 2\delta_{\rho}$ and $n > n_{\rho}$ we obtain

$$P(\hat{d}(\mathbf{x}_i, \mathbf{x}_j) < \delta) \le 2\gamma_{n/2}(\varepsilon_{\rho}). \tag{32}$$

Algorithm 3 produces correct results if for every pair i, j we have $d(\mathbf{x}_i, \mathbf{x}_j) < \delta_n$ if and only if $i, j \in \mathcal{G}_k \cap 1..N$ for some $k \in 1..\kappa$. Therefore, taking the bounds (29) and (32) together for each of the N(N+1)/2 pairs of samples, we obtain (26).

For the online setting, consider the following simple extension of Algorithm 3, that we call Algorithm 3'. It applies Algorithm 3 to the first N_t sequences, where the parameters of Algorithm 3 and N_t are chosen in such a way that the bound (26) with $N=N_t$ is o(1) and $N_t \to \infty$ as time t goes to infinity. It then assigns each of the remaining sequences $(\mathbf{x_i}, i > N_t)$ to the nearest cluster. Note that in this case the bound (26) with $N=N_t$ bounds the error of Algorithm 3' on the first N_t sequences, as long as all of the κ clusters are already represented among the first N_t sequences. Since $N_t \to \infty$, we can formulate the following result.

Theorem 14 Algorithm 3' is weakly asymptotically consistent in the online setting when the number κ of clusters is unknown, provided that the assumptions of Theorem 13 apply to the first N sequences $\mathbf{x}_1, \ldots, \mathbf{x}_N$ for every $N \in \mathbb{N}$.

4.4 Extensions

In this section we show that some simple, yet rather general extensions of the main results of this paper are possible, namely allowing for non-stationarity and for slight differences in distributions in the same cluster.

4.4.1 AMS Processes and Gradual Changes

Here we argue that our results can be strengthened to a more general case where the process distributions that generate the data are Asymptotically Mean Stationary (AMS) ergodic. Throughout the paper we have been concerned with stationary ergodic process distributions. Recall from Section 2 that a process ρ is stationary if for any $i, j \in 1..n$ and $B \in B^m$, $m \in \mathbb{N}$, we have $\rho(X_{1...j} \in B) = \rho(X_{i...i+j-1} \in B)$. A stationary process is called ergodic if the limiting frequencies converge to their corresponding probabilities, so that for all $B \in \mathcal{B}$ with probability 1 we have $\lim_{n\to\infty} \nu(X_{1..n}, B) = \rho(B)$. This latter convergence of all frequencies is the only property of the process distributions that is used in the proofs (via Lemma 5) which give rise to our consistency results. We observe that this property also holds for a more general class of processes, namely those that are AMS ergodic. Specifically, a process ρ is called AMS if for every $j \in 1..n$ and $B \in B^m, m$ N the series $\lim_{n\to\infty}\sum_{i=1}^{n-j+1}\frac{1}{n}\rho(X_{i...i+j-1}\in B)$ converges to a limit $\bar{\rho}(B)$, which forms a measure, i.e. $\bar{\rho}(X_{1...j} \in B) := \bar{\rho}(B), B \in B^m, m \in \mathbb{N}$, called asymptotic mean of ρ . Moreover, if ρ is an AMS process, then for every $B \in B^m$, $m \in \mathbb{N}$, the frequency $\nu(X_{1..n}, B)$ converges ρ -a.s. to a random variable with mean $\bar{\rho}(B)$. Similarly to stationary processes, if the random variable to which $\nu(X_{1..n}, B)$ converges is a.s. constant, then ρ is called AMS ergodic. More information on AMS processes can be found in the work (Gray, 1988). However, the main characteristic pertaining to our work is that the class of all processes with AMS properties is composed precisely of those processes for which the almost sure convergence of frequencies to the corresponding probabilities holds. It is thus easy to check that all of the asymptotic results of Sections 4.1, 4.2 carry over to the more general setting where the unknown process distributions that generate the data are AMS ergodic.

4.4.2 Strictly Separated Clusters of Distributions

So far we have defined a cluster as a set of sequences generated by the same distribution. This seems to capture rather well the notion that in the same cluster the objects can be very different (as is the case for stochastically generated sequences), yet are intrinsically of the same nature (they have the same law).

However, one may wish to generalise this further, and allow each sequence to be generated by a different distribution, yet requiring that in the same clusters distributions must be close. Unlike the original formulation, such an extension would require fixing some similarity measure between distributions. The results of the preceding sections suggest using the distributional distance for this purpose.

Specifically, as discussed in Section 4.1, in our formulation, from some time on, the sequences possess the so-called strict separation property in the \hat{d} distance: sequences in the same target cluster are closer to each other than to those in other clusters. One possible way to relax the considered setting is to impose the strict separation property on the distributions that generate the data. Here the separation would be with respect to the distributional distance d. That is, each sequence $\mathbf{x}_i, i = 1..N$, may be generated by its own distribution ρ_i , but the distributions $\{\rho_i : i = 1..N\}$ can be clustered in such a way that the resulting clustering has the strict separation property with respect to d. The goal would then be to recover this clustering based on the given samples. In fact, it can be shown that the offline Algorithm 1 of Section 4.1 is consistent in this setting as well. How this transfers

to the online setting remains open. For the offline case, we can formulate the following result, whose proof is analogous to that of Theorem 11.

Theorem 15 Assume that each sequence \mathbf{x}_i , i = 1..N is generated by a stationary ergodic distribution ρ_i . Assume further that the set of distributions $\{1, \ldots, N\}$ admits a partitioning $\mathcal{G} = \{\mathcal{G}_1, \ldots, \mathcal{G}_k\}$ that has the strict separation property with respect to d: for all $i, j = 1..k, i \neq j$, for all $\rho_1, \rho_2 \in \mathcal{G}_i$ and all $\rho_3 \in \mathcal{G}_j$ we have $d(\rho_1, \rho_2) < d(\rho_1, \rho_3)$. Then Algorithm 1 is strongly asymptotically consistent, in the sense that almost surely from some $n = \min\{n_1, \ldots, n_N\}$ on it outputs the set \mathcal{G} .

5. Computational Considerations

In this section we show that all of the proposed methods are efficiently computable. This claim is further illustrated by the experimental results in the next section. Note, however, that since the results presented are asymptotic, the question of what is the best achievable computational complexity of an algorithm that still has the same asymptotic performance guarantees is meaningless: for example, an algorithm could throw away most of the data and still be asymptotically consistent. This is why we do not attempt to find a resource-optimal way of computing the methods presented.

First, we show that calculating \hat{d} is at most quadratic (up to log terms), and quasilinear if we use $m_n = \log n$. Let us begin by showing that calculating \hat{d} is fully tractable with $m_n, l_n \equiv \infty$. First, observe that for fixed m and l, the sum

$$T^{m,l} := \sum_{B \in B^{m,l}} |\nu(X_{1..n_1}^1, B) - \nu(X_{1..n_2}^2, B)|$$
(33)

has not more than $n_1 + n_2 - 2m + 2$ nonzero terms (assuming $m \le n_1, n_2$; the other case is obvious). Indeed, there are $n_i - m + 1$ tuples of size m in each sequence \mathbf{x}_i , i = 1, 2 namely, $X_{1...m}^i, X_{2...m+1}^i, \dots, X_{n_1-m+1..n_1}^i$. Therefore, $T^{m,l}$ can be obtained by a finite number of calculations.

Furthermore, let

$$s = \min_{\substack{X_i^1 \neq X_j^2 \\ i=1..n_1, j=1..n_2}} |X_i^1 - X_j^2|, \tag{34}$$

and observe that $T^{m,l} = 0$ for all m > n and for each m, for all $l > \log s^{-1}$ the term $T^{m,l}$ is constant. That is, for each fixed m we have

$$\sum_{l=1}^{\infty} w_m w_l T^{m,l} = w_m w_{\log s^{-1}} T^{m,\log s^{-1}} + \sum_{l=1}^{\log s^{-1}} w_m w_l T^{m,l}$$

so that we simply double the weight of the last nonzero term. (Note also that s is bounded above by the length of the binary precision in representing the random variables X_j^i .) Thus, even with $m_n, l_n \equiv \infty$ one can calculate \hat{d} precisely. Moreover, for a fixed $m \in 1$.. $\log n$ and $l \in 1$.. $\log s^{-1}$ for every sequence \mathbf{x}_i , i = 1, 2 the frequencies $\nu(\mathbf{x}_i, B)$, $B \in B^{m,l}$ may be calculated using suffix trees or suffix arrays, with $\mathcal{O}(n)$ worst case construction and search complexity (see, e.g., Ukkonen, 1995). Searching all z := n - m + 1 occurrences of

subsequences of length m results in $\mathcal{O}(m+z) = \mathcal{O}(n)$ complexity. This brings the overall computational complexity of (3) to $\mathcal{O}(nm_n \log s^{-1})$; this can potentially be improved using specialized structures, e.g., (Grossi and Vitter, 2005).

The following consideration can be used to set m_n . For a fixed l the frequencies $\nu(\mathbf{x}_i, B)$, i=1,2 of cells in $B \in B^{m,l}$ corresponding to values of m much larger than \log_n (in the asymptotic sense, that is, if $\log_n = o(m)$) are not, in general, consistent estimates of their probabilities, and thus only add to the estimation error. More specifically, for a subsequence $X_{j..j+m}$ with j=1..n-m of length m the probability $\rho_i(X_{j..j+m} \in B)$, i=1,2 is of order 2^{-mh_i} , i=1,2 where h_i denotes the entropy rate of ρ_i , i=1,2. Moreover, under some (general) conditions (including $h_i > 0$) one can show that, asymptotically, a string of length of order $\log n/h_i$ on average occurs at most once in a string of length n (Kontoyiannis and Suhov, 1994). Therefore, subsequences of length m larger than $\log n$ are typically met 0 or 1 times, and thus are not consistent estimates of probabilities. By the above argument, one can use m_n of order $\log n$. To choose $l_n < \infty$ one can either fix some constant based on the bound on the precision in real computations, or choose it in such a way that each cell B^{m,l_n} contains no more than $\log n$ points for all m=1.. $\log n$ largest values of l_n .

5.1 Complexity of the Algorithms.

The computational complexity of the presented algorithms is dominated by the complexity of calculations of \hat{d} between different pairs of sequences. Thus, it is sufficient to bound the number of pairwise \hat{d} computations.

It is easy to see that the offline algorithm for the case of known κ (Algorithm 1) requires at most κN distance calculations, while for the case of unknown κ all N^2 distance calculations are necessary.

The computational complexity of the updates in the online algorithm can be computed as follows. Assume that the pairwise distance values are stored in a database D, and that for every sequence \mathbf{x}_i^{t-1} , $i \in \mathbb{N}$ we have already constructed a suffix tree, using for example, the online algorithm of Ukkonen (1995). At time step t, a new symbol X is received. Let us first calculate the required computations to update D. We have two cases, either X forms a new sequence, so that N(t) = N(t-1) + 1, or it is the subsequent element of a previously received segment, say, \mathbf{x}_j^t for some $j \in 1..N(t)$, so that $n_j(t) = n_j(t-1) + 1$. In either case, let \mathbf{x}_j^t denote the updated sequence. Note that for all $i \neq j \in 1..N(t)$ we have $n_i(t) = n_i(t-1)$. Recall the notation $\mathbf{x}_i^t := X_1^{(i)}, \ldots X_{n_i(t)}^{(i)}$ for $i \in 1..N(t)$. In order to update D we need to update the distance between \mathbf{x}_j^t and \mathbf{x}_i^t for all $i \neq j \in N(t)$. Thus, we need to search for all m_n new patterns induced by the received symbol X, resulting in complexity at most $\mathcal{O}(N(t)m_n^2l_n)$. Let $n(t) := \max\{n_1(t), \ldots n_{N(t)}(t)\}$, $t \in \mathbb{N}$. As discussed previously, we let $m_n := \log n(t)$; we also define $l_n := \log s(t)^{-1}$ where

$$s(t) := \min_{\substack{i,j \in 1..N(t) \\ u = 1..n_i(t), v = 1..n_j(t), X_u^{(i)} \neq X_v^{(j)}}} |X_u^{(i)} - X_v^{(j)}|, \ t \in \mathbb{N}.$$

Thus, the per symbol complexity of updating D is at most $\mathcal{O}(N(t)\log^3 n(t))$. However, note that if s(t) decreases from one time step to the next, updating D will have a complexity

of order equivalent to its complete construction, resulting in a computational complexity of order $\mathcal{O}(N(t)n(t)\log^2 n(t))$. Therefore, we avoid calculating s(t) at every time step; instead, we update s(t) at prespecified time steps so that for every n(t) symbols received, D is reconstructed at most $\log n(t)$ times. (This can be done, for example, by recalculating s(t) at time steps where n(t) is a power of 2.) It is easy to see that with the database D of distance values at hand, the rest of the computations are of order at most $\mathcal{O}(N(t)^2)$. Thus, the computational complexity of updates in Algorithm 2 is at most $\mathcal{O}(N(t)^2+N(t)\log^3 n(t))$.

6. Experimental Results

In this section we present empirical evaluations of Algorithms 1 and 2 on both synthetically generated and real data.

6.1 Synthetic Data

We start with synthetic experiments. In order for the experiments to reflect the generality of our approach we have selected time-series distributions that, while being stationary ergodic, cannot be considered as part of any of the usual smaller classes of processes, and are difficult to approximate by finite-state models. Namely, we consider rotation processes used, for example, by Shields (1996) as an example of stationary ergodic processes that are not B-processes. Such time series cannot be modelled by a hidden Markov model with a finite or countably infinite set of states. Moreover, while k-order Markov (or hidden Markov) approximations of this process converge to it in the distributional distance d, they do not converge to it in the \bar{d} distance, a stronger distance than d whose empirical approximations are often used to study general (non-Markovian) processes (e.g., Ornstein and Weiss, 1990).

6.1.1 Time Series Generation

To generate a sequence $\mathbf{x} = X_{1..n}$ we proceed as follows: Fix some parameter $\alpha \in (0,1)$. Select $r_0 \in [0,1]$; then, for each i=1..n obtain r_i by shifting r_{i-1} by α to the right, and removing the integer part, i.e. $r_i := r_{i-1} + \alpha - \lfloor r_{i-1} + \alpha \rfloor$. The sequence $\mathbf{x} = (X_1, X_2, \cdots)$ is then obtained from r_i by thresholding at 0.5, that is $X_i := \mathbb{I}\{r_i > 0.5\}$. If α is irrational then \mathbf{x} forms a stationary ergodic time series. (We simulate α by a longdouble with a long mantissa.)

For the purpose of our experiments, first we fix $\kappa := 5$ difference process distributions specified by $\alpha_1 = 0.31...$, $\alpha_2 = 0.33...$, $\alpha_3 = 0.35...$, $\alpha_4 = 0.37...$, $\alpha_5 = 0.39...$ The parameters α_i are intentionally selected to be close, in order to make the process distributions harder to distinguish. Next we generate an $N \times M$ data matrix \mathbf{X} , each row of which is a sequence generated by one of the process distributions. Our task in both the online and the batch setting is to cluster the rows of \mathbf{X} into $\kappa = 5$ clusters.

6.1.2 Batch Setting

In this experiment we demonstrate that in the batch setting, the clustering errors corresponding to both the online and the offline algorithms converge to 0 as the sequence-lengths grow. To this end, at every time step t we take an $N \times n(t)$ submatrix $\mathbf{X}|_{\mathbf{n(t)}}$ of \mathbf{X} composed of the rows of \mathbf{X} terminated at length n(t), where n(t) = 5t. Then at each iteration we let

each of the algorithms, (online and offline) cluster the rows of $\mathbf{X}|_{\mathbf{n(t)}}$ into five clusters, and calculate the clustering error rate of each algorithm. As shown in Figure 2 (top) the error rate of each algorithm decreases with sequence length.

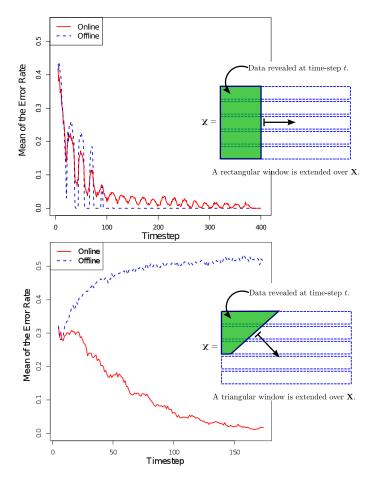


Figure 2: Top: error rate vs. sequence length in batch setting. Bottom: error rate vs. Number of observed samples in online setting. (error rates averaged over 100 runs.)

6.1.3 Online Setting

In this experiment we demonstrate that, unlike the online algorithm, the offline algorithm is consistently confused by the new sequences arriving at each time step in an online setting. To simulate an online setting, we proceed as follows: At every time step t, a triangular window is used to reveal the first $1..n_i(t)$, i = 1..t elements of the first t rows of the data matrix \mathbf{X} , with $n_i(t) := 5(t-i) + 1$, i = 1..t. This gives a total of t sequences, each of length $n_i(t)$, for i = 1..t, where the i^{th} sequence for i = 1..t corresponds to the i^{th} row of \mathbf{X} terminated at length $n_i(t)$. At every time step t the online and offline algorithms are each used in turn to cluster the observed t sequences into five clusters. Note that the performance

of both algorithms is measured on all sequences available at a given time, not on a fixed batch of sequences. As shown in Figure 2 (bottom), in this setting the clustering error rate of the offline algorithm remains consistently high, whereas that of the online algorithm converges to zero.

6.2 Real Data

As an application we consider the problem of clustering motion capture sequences, where groups of sequences with similar dynamics are to be identified. Data is taken from the Motion Capture database (MOCAP) which consists of time-series data representing human locomotion. The sequences are composed of marker positions on human body which are tracked spatially through time for various activities.

We compare our results to those obtained with two other methods, namely those of Li and Prakash (2011) and Jebara et al. (2007). Note that we have not implemented these reference methods, rather we have taken the numerical results directly from the corresponding articles. In order to have common grounds for each comparison we use the same sets of sequences² and the same means of evaluation as those used by Li and Prakash (2011); Jebara et al. (2007).

In the paper by Li and Prakash (2011) two MOCAP data sets³ are used, where the sequences in each data set are labelled with either running or walking as annotated in the database. Performance is evaluated via the conditional entropy S of the true labelling with respect to the prediction, i.e., $S := -\sum_{i,j} \frac{\mathcal{M}_{ij}}{\sum_{i',j'} \mathcal{M}_{i'j'}} \log \frac{\mathcal{M}_{ij}}{\sum_{j'} \mathcal{M}_{ij'}}$ where \mathcal{M} denotes the clustering confusion matrix. The motion sequences used by Li and Prakash (2011) are reportedly trimmed to equal duration. However, we use the original sequences as our method is not limited by variation in sequence lengths. Table 1 lists performance of Algorithm 1 as well as that reported for the method of Li and Prakash (2011); Algorithm 1 performs consistently better.

In the paper (Jebara et al., 2007) four MOCAP data sets⁴ are used, corresponding to four motions: run, walk, jump and forward jump. Table 2 lists performance in terms of accuracy. The data sets in Table 2 constitute two types of motions:

- 1. motions that can be considered ergodic: walk, run, run/jog (displayed above the double line), and
- 2. non-ergodic motions: single jumps (displayed below the double line).

As shown in Table 2, Algorithm 1 achieves consistently better performance on the first group of data sets, while being competitive (better on one and worse on the other) on the non-ergodic motions. The time taken to complete each task is in the order of few minutes on a standard laptop computer.

^{2.} The subject's right foot was used as marker position.

^{3.} The corresponding subject references are #16 and #35.

^{4.} The corresponding subject references are #7, #9, #13, #16 and #35.

	Data set	(Li and Prakash, 2011)	Algorithm 1
1.	Walk vs. Run (#35)	0.1015	0
2.	Walk vs. Run (#16)	0.3786	0.2109

Table 1: Comparison with the work (Li and Prakash, 2011): Performance in terms of entropy; data sets concern ergodic motion captures.

	Data set	(Jebara et al., 2007)	Algorithm 1
1.	$\operatorname{Run}(\#9)$ vs. $\operatorname{Run}/\operatorname{Jog}(\#35)$	100%	100%
2.	Walk(#7) vs. $Run/Jog(#35)$	95%	100%
3.	Jump vs. Jump fwd.(#13)	87%	100%
4.	Jump vs. Jump fwd.(#13, 16)	66 %	60%

Table 2: Comparison with the work (Jebara et al., 2007): Performance in terms of accuracy; Rows 1 & 2 concern ergodic, Rows 3 & 4 concern non-ergodic motion captures.

7. Discussion

We have proposed a natural notion of consistency for clustering time series in both the online and the offline settings. While in this work we have taken some first steps in investigating the theoretical and algorithmic questions arising in the proposed framework, there are many open problems and exciting directions for future research remaining to be explored. Some of these are discussed in this section.

Rates, optimality. The main focus of this work is on the most general case of highly dependent time series. On the one hand, this captures best the spirit of the unsupervised learning problem in question: the nature of the data is completely unknown, and one tries to find some structure in it. On the other hand, as discussed above, in this generality rates of convergence and finite-sample performance guarantees are provably impossible to obtain, and thus one cannot argue about optimality. While we have provided some results on a more restrictive setting (time series with mixing, Section 4.3), the question of what the optimal performance guarantees are for different classes of time series remains open. In fact, the first interesting question in this direction is not about time series with mixing, but about i.i.d. series. What is the minimal achievable probability of clustering error in this setting, for finite sample sizes, and what algorithms attain it?

Online setting: bad points. In the online setting of Section 4.2, we have assumed that the length of each sequence grows to infinity with time. While this is a good first approximation, this assumption may not be practical. It is interesting to consider the situation in which some sequences stop growing at some point; moreover, it can be assumed that such sequences are not representative of the corresponding distribution. While this clearly makes the problem much more difficult, already in the setting considered in this work we have dealt with "bad" sequences at each time step: these are those sequences which are as yet too short to be informative. This hints at the possibility of obtaining consistent algorithms in the extended setting outlined.

Other metrics and non-metric-based methods. All of the methods presented in this paper are based on the distributional distance d. The main property of this distance that we

exploit is that it can be estimated consistently. In principle, one can use other distances with this property, in order to obtain consistent clustering algorithms. While there are not many known distances that can be consistently estimated for arbitrary stationary ergodic distributions, there is at least one, namely the telescope distance recently introduced by Ryabko and Mary (2013). Moreover, the definition of consistency proposed does not entail the need to use a distance between time-series distributions. As an alternative, the use of compression-based methods can be considered. Such methods have been used to solve various statistical problems concerning stationary ergodic time series (Ryabko and Astola, 2006; Ryabko, 2010a). Compression-based methods have also been used for clustering time-series data before, albeit without consistency analysis, by Cilibrasi and Vitanyi (2005). Combining our consistency framework with these compression-based methods is another promising direction for further research.

Acknowledgments

This paper is an extended version of two conference papers: (Ryabko, 2010b) and (Khaleghi et al., 2012). Most of the work by Azadeh Khaleghi has been done during her PhD at INRIA Lille - Nord Europe. This work is supported by the French Ministry of Higher Education and Research, by FP7/2007-2013 under grant agreements 270327 (CompLACS), by the Nord-Pas-de-Calais Regional Council and FEDER, and by the European Research Council (SMAC-ERC-280032). Jérémie Mary and Philippe Preux acknowledge the support of INRIA. Jérémie Mary further acknowledges INRIA for the support through partial secondments.

References

- F.R. Bach and M.I. Jordan. Learning graphical models for stationary time series. *IEEE Transactions on Signal Processing*, 52(8):2189 2199, Aug. 2004.
- M.F. Balcan, A. Blum, and S. Vempala. A discriminative framework for clustering via similarity functions. In *Proceedings of the 40th Annual ACM Symposium on Theory of Computing*, pages 671–680, 2008.
- C. Biernacki, G. Celeux, and G. Govaert. Assessing a mixture model for clustering with the integrated completed likelihood. *Pattern Analysis and Machine Intelligence*, *IEEE Transactions on*, 22(7):719–725, 2000.
- P. Billingsley. Statistical methods in Markov chains. *The Annals of Mathematical Statistics*, 32(1):12–40, 1961.
- P. Billingsley. Convergence of Probability Measures. John Wiley & Sons, 1999.
- D. Bosq. Nonparametric Statistics for Stochastic Processes. Estimation and Prediction. Springer, 1996.
- R.C. Bradley. Basic properties of strong mixing conditions: A survey and some open questions. *Probability Surveys*, 2:107–144, 2005.

- E. Carlstein and S. Lele. Nonparametric change-point estimation for data from an ergodic sequence. Theory of Probability & its Applications, 38(4):726–733, 1994.
- N. Cesa-Bianchi and G. Lugosi. Prediction, Learning, and Games. Cambridge University Press, 2006.
- R. Cilibrasi and P.M.B. Vitanyi. Clustering by compression. *IEEE Transactions on Information Theory*, 51:1523–1545, 2005.
- P. Doukhan. Mixing. Springer, 1994.
- P. Doukhan, G. Lang, D. Surgailis, and G. Teyssière. Dependence in Probability and Statistics. Springer, 2010.
- R. Gray. Probability, Random Processes, and Ergodic Properties. Springer Verlag, 1988.
- R. Grossi and J.S. Vitter. Compressed suffix arrays and suffix trees with applications to text indexing and string matching. SIAM Journal on Computing, 35(2):378–407, 2005.
- M. Gutman. Asymptotically optimal classification for multiple tests with empirically observed statistics. *IEEE Transactions on Information Theory*, 35(2):402–408, 1989.
- T. Jebara, Y. Song, and K. Thadani. Spectral clustering and embedding with hidden Markov models. *Machine Learning: ECML 2007*, pages 164–175, 2007.
- I. Katsavounidis, C.-C. Jay Kuo, and Zhen Zhang. A new initialisation technique for generalised Lloyd iteration. *IEEE Signal Processing Letters*, 1:144–146, 1994.
- A. Khaleghi and D. Ryabko. Locating changes in highly-dependent data with unknown number of change points. In *Neural Information Processing Systems (NIPS)*, Lake Tahoe, Nevada, United States, 2012.
- A. Khaleghi, D. Ryabko, J. Mary, and P. Preux. Online clustering of processes. In *International Conference on Artificial Intelligence and Statistics (AI&STATS)*, JMLR W&CP 22, pages 601–609, 2012.
- A. Khaleghi and D. Ryabko. Asymptotically consistent estimation of the number of change points in highly dependent time series. In the Proceedings of the 29th International Conference on Machine Learning (ICML), JMLR W&CP, pages 539–547, Beijing, China, 2014.
- J. Kleinberg. An impossibility theorem for clustering. In *Neural Information Processing Systems (NIPS)*, pages 446–453, Montreal, Canada, 2002.
- I. Kontoyiannis and Y.M. Suhov. Prefixes and the entropy rate for long-range sources. In *IEEE International Symposium on Information Theory*, pages 194–194, 1994.
- M. Kumar, N.R. Patel, and J. Woo. Clustering seasonality patterns in the presence of errors. In *Proceedings of the 8th International Conference on Knowledge Discovery and Data Mining (ACM SIGKDD)*, pages 557–563. ACM, 2002.

- E. Lehmann. Testing Statistical Hypotheses, 2nd edition. Wiley, New York, 1986.
- L. Li and B.A. Prakash. Time series clustering: Complex is simpler! In the Proceedings of the 28th International Conference on Machine Learning (ICML), pages 185–192, 2011.
- M. Mahajan, P. Nimbhorkar, and K. Varadarajan. The planar k-means problem is NP-hard. In the Proceedings of the 3rd International Workshop on Algorithms and Computation (WALCOM), pages 274–285, Berlin, Heidelberg, 2009.
- G. Morvai and B. Weiss. On classifying processes. Bernoulli, 11(3):523–532, 2005.
- MOCAP. CMU graphics lab motion capture database. Available at http://mocap.cs.cmu.edu/.
- G. Morvai and B. Weiss. A note on prediction for discrete time series. *Kybernetika*, 48(4): 809–823, 2012.
- D.S. Ornstein and B. Weiss. How sampling reveals a process. *Annals of Probability*, 18(3): 905–930, 1990.
- E. Rio. Théorie asymptotique des processus aléatoires faiblement dépendants, volume 31. Springer, 1999.
- B. Ryabko. Prediction of random sequences and universal coding. *Problems of Information Transmission*, 24:87–96, 1988.
- B. Ryabko and J. Astola. Universal codes as a basis for time series testing. *Statistical Methodology*, 3:375–397, 2006.
- B. Ryabko. Applications of universal source coding to statistical analysis of time series. Selected Topics in Information and Coding Theory, World Scientific Publishing, pages 289–338, 2010a.
- D. Ryabko. Clustering processes. In the Proceedings of the 27th International Conference on Machine Learning (ICML), pages 919–926, Haifa, Israel, 2010b.
- D. Ryabko. Discrimination between B-processes is impossible. Journal of Theoretical Probability, 23(2):565–575, 2010c.
- D. Ryabko. Testing composite hypotheses about discrete ergodic processes. *Test*, 21(2): 317–329, 2012.
- D. Ryabko. Uniform hypothesis testing for finite-valued stationary processes. *Statistics*, 48 (1):121–128, 2014.
- D. Ryabko and B. Ryabko. Nonparametric statistical inference for ergodic processes. *IEEE Transactions on Information Theory*, 56(3):1430–1435, 2010.
- D. Ryabko and J. Mary. A binary-classification-based metric between time-series distributions and its use in statistical and learning problems. *Journal of Machine Learning Research*, 14:2837–2856, 2013.

KHALEGHI, RYABKO, MARY AND PREUX

- P. Shields. The Ergodic Theory of Discrete Sample Paths. AMS Bookstore, 1996.
- P. Smyth. Clustering sequences with hidden Markov models. In *Advances in Neural Information Processing Systems*, pages 648–654. MIT Press, 1997.
- M. Tschannen and H. Bolcskei. Nonparametric nearest neighbor random process clustering. In *Proceedings of the 2015 IEEE International Symposium on Information Theory*, pages 1207–1211, Hong Kong, 2015. IEEE.
- E. Ukkonen. On-line construction of suffix trees. Algorithmica, 14(3):249–260, 1995.
- S. Zhong and J. Ghosh. A unified framework for model-based clustering. *Journal of Machine Learning Research*, 4:1001–1037, 2003.