An RPCL-Based Approach for Markov Model Identification with Unknown State Number

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***Abstract*—This paper presents an alternative identification approach for the Markov model studied in [3]. Our approach estimates the state sequence and model parameters with the help of a clustering analysis by the rival penalized competitive learning (RPCL) algorithm [4]. Compared to the method in [3], this new approach not only extends the model from scalar states to multidimensional ones, but also makes the model identification with the correct number of states decided automatically. The experiments have shown that it works well.**

***Index Terms*—Clustering property, Markov model identification, number of states, rival penalized competitive learning (RPCL).**

I. Introduction

RECENTLY, one Markov model has been studied in paper [3] due to its attractive applications in neurobiological signal processing and communication systems. This model formulates a discrete time finite-scalar-state Markov chain observed under the corruption of noise. Paper [3] has presented an on-line EM algorithm based on the Kullback–Leibler information measure to identify the model's parameters and state sequence. The experiments in [3] have shown that this on-line EM-based algorithm can significantly reduce memory requirements and improve EM convergence in contrast to the off-line EM algorithms [1], [2]. However, this approach assumes that the number of states is exactly known in advance, otherwise its performance may deteriorate to a certain degree. Unfortunately, this assumption is often violated in practice, leaving the estimation of the number of states as an open practical problem.

In this paper, we extend the above model from scalar states to multidimensional ones, and present an alternative approach to identify the model with unknown number of states. We will show in Section III that the observations from the model form a set of clusters, each of which corresponds to noisy observations of a state. That is, the number of states is equal to the number of clusters. Hence, our proposed approach first estimates the state number by using the rival penalized competitive learning (RPCL) Type B algorithm [6], [5], which is robust in automatically finding out the correct cluster number while performing clustering. Then the state sequence is recovered by Bayesian decision via a variant of the EM algorithm [4] and the model parameters are estimated. The experiment performed has shown that this new approach works well.

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II. Markov Model Identification Problem

Let $\mathbf{s}_t$ be a finite state, discrete-time, first order irreducible ergodic Markov process. At each time t, $\mathbf{s}_t$ is one of k finite states $\mathbf{q}_j \in \mathbf{Q} = \{\mathbf{q}_j\}_{j=1}^k$ with $\mathbf{q}_j \in \Re^d$. Let the (i, j)th element a_{ij} of the transition probability matrix $\mathbf{A}$ be the conditional transition probability from $\mathbf{q}_i$ to $\mathbf{q}_j$ and denote the stationary probability of $\mathbf{q}_j$ by $\pi_j \in \pi = \{\pi_j\}_{j=1}^k$. The state sequence $\mathbf{s}_1, \cdots, \mathbf{s}_N$ are not directly known but only noisily observed as $\mathbf{x}_1, \cdots, \mathbf{x}_N$. The observation noise are white, zero-mean, and Gaussian but the covariances $\mathbf{\Sigma}_j$'s of noise in observing different states $\mathbf{q}_j$'s are in general different. Therefore, the observation equation can be written as

$$\mathbf{x}_t = \mathbf{s}_t + \mathbf{e}_t^{(j)} \tag{1}$$

where $\mathbf{e}_t^{(j)}$ is observation noise of state $\mathbf{q}_j$ that $\mathbf{s}_t$ is in, and

$$\mathbf{e}_t^{(j)} \sim G\left(\mathbf{e}_t^{(j)} | \mathbf{0}, \mathbf{\Sigma}_j\right) \tag{2}$$

with $G(\mathbf{e}_t^{(j)}|\mathbf{0}, \mathbf{\Sigma}_j)$ denoting the Gaussian distribution of $\mathbf{e}_t^{(j)}$ with mean $\mathbf{0}$ and covariance matrix $\mathbf{\Sigma}_j$.

In this model, k, $\mathbf{Q}$, $\{\mathbf{\Sigma}_j\}_{j=1}^k$, $\mathbf{A}$, π, and the state sequence $\mathbf{s}_1, \cdots, \mathbf{s}_N$ are all unknown and only the observation sequence $\mathbf{x}_1, \cdots, \mathbf{x}_N$ is known. The problem is to identify all the above mentioned unknown quantities from the observation sequence alone.

III. New Approach to the Problem

The unknown quantities to be identified can be classified into two categories. The first category, consisting of k, $\mathbf{Q}$, $\{\mathbf{\Sigma}_j\}_{j=1}^k$, and π, is related only to some properties of the observation data set $D = \{\mathbf{x}_t\}_{t=1}^N$ without regarding the temporal relationship between the data points. The second category consists of the transition probability matrix $\mathbf{A}$ and state sequence $\mathbf{s}_1, \cdots, \mathbf{s}_N$ that are related to the temporal relationship along the observation sequence.

The identification of the unknowns in the first category is based on the insight that they are not relevant to the temporal relationship, and therefore, we can drop the temporal meaning of the time index of the observation sequence at this stage. In the observation space, from (2), the noisy observations $\mathbf{x}_t$'s of $\mathbf{s}_t = \mathbf{q}_j$ are samples from the distribution $G(\mathbf{x}|\mathbf{q}_j, \mathbf{\Sigma}_j)$. Since π_j is the stationary probability that a realization of $\mathbf{s}_t$ happens to be $\mathbf{q}_j$ without regarding the temporal relationship, the whole

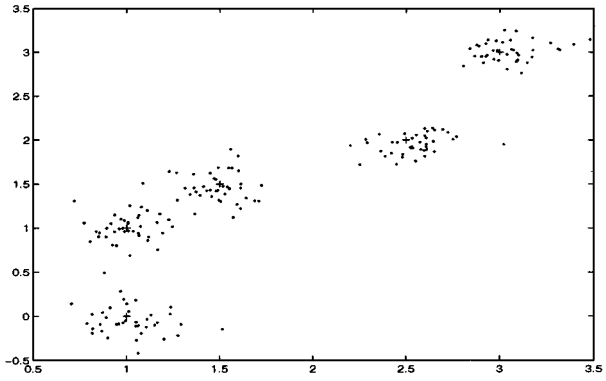

Fig. 1. Two-dimensional (2-D) example demonstrating that the observations of the Markov process (1), with five states marked by "+," form five visible clusters.

observation data set D can be regarded as samples from the following mixture of Gaussians

$$p(\mathbf{x}) = \sum_{j=1}^{k} \pi_j G(\mathbf{x}\,|\mathbf{q}_j, \boldsymbol{\Sigma}_j)\,. \tag{3}$$

Samples from a mixture-of-Gaussians generally form a set of clusters. Fig. 1 shows an example that the observations of the Markov process form clusters. In this correspondence between noisy observations of a state $\mathbf{q}_j$ and a cluster that we call C_j, we can identify k as the determined number of clusters in the observation space k. Up to a nonidentifiable permutation of index j, $\mathbf{Q}$, $\{\boldsymbol{\Sigma}_j\}_{j=1}^{k}$, and π can be estimated as the cluster centers, cluster covariances, and the relative numbers of data points in the clusters.

The parameters of the clusters can be estimated by the well known maximum likelihood (ML) approach with the EM algorithm, and an appropriate k can be determined by the number selection criteria recently proposed in [4]. However, the computational procedure in [4] can be laborious. Therefore, in this paper we propose using a more simple and intuitive heuristic method called rival penalized competitive learning (RPCL) Type B clustering algorithm [6], [5], which showed the best performance in selecting the correct k in previous studies [5], to automatically determine an appropriate number of clusters $\hat{k}$. Then, the observation points are classified into the $\hat{k}$ clusters according to Bayesian (maximum *a posteriori* probability: MAP) decision simultaneously with cluster centers, covariances,and stationary probabilities estimated by a variant of the EM algorithm called the "hard-cut" EM algorithm [4], which converges faster than the EM algorithm.

After the unknowns of the first category are identified, each state $\mathbf{s}_t$ can be easily recovered as the $\mathbf{q}_j$ corresponding to the cluster C_j that $\mathbf{x}_t$ classified into. Finally, we identify $\mathbf{A}$ according to the transition frequency of the estimated $\mathbf{s}_t$ from one state to another one. In the next section, we will go into details of the algorithm.

IV. Algorithm of the RPCL-Based Approach for Markov Model Identification

Given an observation sequence $\mathbf{x}_1, \cdots, \mathbf{x}_N$, our proposed RPCL-based approach consists of two stages. In Stage 1, we use the RPCL Type B algorithm [5] to estimate the number of states k and give preliminary estimates of cluster centers, covariances, and proportions as initial values of the iterative algorithm in Stage 2. In Stage 2, we use the hard-cut EM algorithm [4] to estimate $\mathbf{Q}$, $\{\boldsymbol{\Sigma}_j\}_{j=1}^{k}$, and π, then recover $\mathbf{s}_1, \cdots, \mathbf{s}_N$ and estimate $\mathbf{A}$.

Stage 1: RPCL Clustering and Identification of k

Please read papers [6], [5] for details of the algorithm. Here, we only show how we use algorithm in our problem.

Step 1: **Initialization**: Randomly place n ($n \geq k$) *seed points* $\{\mathbf{w}_j\}_{j=1}^{n}$ in the observation space containing the data set D with n appropriately determined either from a prior information on k or by simply setting n large enough. $\hat{\boldsymbol{\Sigma}}_j$'s can be initialized as any positive definite matrix. We initialize the *counts of winning* $m_j = 1, j = 1, \cdots, n$ and approximate $\hat{\pi}_j$ by

$$\hat{\pi}_j = m_j / \sum_i m_i. \tag{4}$$

Step 2: **Adaptive learning**:

Sequentially, take the observation $\mathbf{x}_t$ from the data set D. For each $\mathbf{x}_t$, determine the *winner* seed point $\mathbf{w}_{c(t)}$ and the *rival* seed point $\mathbf{w}_{r(t)}$ according to

$$\begin{aligned} c(t) &= \arg \min_{1 \leq j \leq n} d_j(t) \\ r(t) &= \arg \min_{j \neq c,\, 1 \leq j \leq n} d_j(t) \\ d_j(t) &= \hat{\pi}_j \left[(\mathbf{x}_t - \mathbf{w}_j)^T \hat{\boldsymbol{\Sigma}}_j^{-1} (\mathbf{x}_t - \mathbf{w}_j) + \ln \left| \hat{\boldsymbol{\Sigma}}_j \right| \right]. \end{aligned} \tag{5}$$

The winner is moved in a direction that increases the posterior probability that $\mathbf{x}_t$ belongs to $C_{c(t)}$, $P(c(t)|\mathbf{x}_t)$, and rival is moved in a direction that decreases $P(r(t)|\mathbf{x}_t)$. That is

$$\mathbf{w}_j^{new} = \mathbf{w}_j^{old} + \Delta \mathbf{w}_j(t) \tag{6}$$

with

$$\Delta \mathbf{w}_j(t) = \begin{cases} \alpha_c \boldsymbol{\Sigma}_c^{-1} (\mathbf{x}_t - \mathbf{w}_j^{old}), & \text{if } j = c(t) \\ -\alpha_r \boldsymbol{\Sigma}_r^{-1} (\mathbf{x}_t - \mathbf{w}_j^{old}), & \text{if } j = r(t) \\ 0 & \text{otherwise} \end{cases}$$

where α_c and α_r with $0 < \alpha_r \ll \alpha_c < 1$ are the learning rates for the winner and rival, respectively. We use fixed learning rates during the whole process for practicality. The covariance of the winner's cluster is adaptively learned by

$$\hat{\boldsymbol{\Sigma}}_c^{new} = (1 - \alpha_c) \hat{\boldsymbol{\Sigma}}_c^{old} + \alpha_c (\mathbf{x}_t - \mathbf{w}_c^{new})(\mathbf{x}_t - \mathbf{w}_c^{new})^T$$

while the covariances of other clusters remain unchanged. The count for winner $m_{c(t)}$ is incremented by 1 and $\hat{\pi}$ is updated according to (4).

Step 2 is repeated until the winner-ship of seed points is unchanged for all $\mathbf{x}_t \in D$. The RPCL Type B algorithm is quite robust in successfully moving an appropriate number of seed points to the small regions around the centers of the clusters and

the other excessive seed points away from the clusters [5]. The seed points converged to the places surrounded by data points are regarded as cluster centers preliminarily, and those diverged away from the data points are regarded as excessive and discarded. The remaining number of seed points is denoted as $\hat{k}$. The number of states k is thus identified as $\hat{k}$ now. We use the remaining $\hat{k}$ seed points as preliminary estimates of $\mathbf{Q}$.

Stage 2: Estimation of State Set, State Sequence and Model Parameters

The RPCL Type B algorithm actually does not provide MAP clustering. The preliminary estimates of cluster parameters are only approximation to those according to MAP clustering. Therefore, after Stage 1, we carry out MAP clustering and estimation of the cluster parameters with the hard-cut EM algorithm [4] as follows.

Step 1: **Bayesian (MAP) classification**: Each $\mathbf{x}_t$ is classified into the C_j with maximum log posterior probability $\ln p(j|\mathbf{x}_t)$ that $\mathbf{x}_t$ is in C_j. We represent the classification with the indicator function $I_j(t)$

$$I_j(t) = \begin{cases} 1, & \text{if } j = \arg\min\limits_{1 \le i \le \hat{k}} d_i'(t) \\ 0, & \text{otherwise} \end{cases} \tag{7}$$

with

$$\begin{aligned} d_i'(t) &= -\ln p(j|\mathbf{x}_t) \\ &= (\mathbf{x}_t - \hat{\mathbf{q}}_i)^T \hat{\mathbf{\Sigma}}_j^{-1} (\mathbf{x}_t - \hat{\mathbf{q}}_j) + \ln \left| \hat{\mathbf{\Sigma}}_j \right| - 2 \ln \hat{\pi}_i + K \end{aligned}$$

where K is an unimportant constant.

Step 2: **Updating of $\mathbf{q}_j$, $\mathbf{\Sigma}_j$, and π**: We recalculate

$$\begin{aligned} \hat{\mathbf{q}}_j &= \frac{1}{N_j} \sum_{t=1}^{N} I_j(t) \mathbf{x}_t, \\ \hat{\mathbf{\Sigma}}_\mathbf{j} &= \frac{1}{N_j} \sum_{t=1}^{N} I_j(t) (\mathbf{x}_t - \hat{\mathbf{q}}_j)(\mathbf{x}_t - \hat{\mathbf{q}}_j)^T \\ \hat{\pi}_j &= \frac{1}{N_j} \sum_{t=1}^{N} I_j(t), \quad N_j = \sum_{t=1}^{N} I_j(t). \end{aligned} \tag{8}$$

The above two steps are iterated until convergence occurs, i.e., the classification of all the $\{\mathbf{x}_t\}_{t=1}^N$ does not change. Since Stage 1 has already provided good initial values to the hard-cut EM algorithm, the number of iterations will generally be small. Now the estimates of $\mathbf{Q}$, $\{\mathbf{\Sigma}_j\}_{j=1}^k$, and π are obtained.

Finally, we estimate the unknowns in the second category.

1) **Recovery of state sequence**: Each $\mathbf{s}_t$ is estimated to be the $\mathbf{q}_j$ with maximum posterior probability from the result obtained above. That is, $\hat{\mathbf{s}}_t = \mathbf{q}_j$, where j is the unique one with $I_j(t) = 1$.
2) **Estimation of $\mathbf{A}$**: The transition probability $a_{i,j}$ can be estimated by counting the relative frequency of transition from $\hat{\mathbf{q}}_i$ to $\hat{\mathbf{q}}_j$ in the $N-1$ pairs of $\hat{\mathbf{s}}_t$ and $\hat{\mathbf{s}}_{t+1}$ in the whole state sequence. In implementation, we initialize a $\hat{k} \times \hat{k}$ matrix $\mathbf{B} = (b_{ij})$ as zero matrix, and then adaptively update the (i, j)th element of $\mathbf{B}$ for each time t by

$$b_{ij} = \begin{cases} b_{ij} + I_j(t+1), & \text{if } \mathbf{x}_t \in C_i, \\ b_{ij}, & \text{otherwise.} \end{cases} \tag{9}$$

Afterward, the transition matrix $\mathbf{A}$ is estimated by $\hat{\mathbf{A}} = (\hat{a}_{ij})$ with

$$\hat{a}_{ij} = \frac{b_{ij}}{\sum\limits_{m=1}^{\hat{k}} b_{im}}. \tag{10}$$

V. Simulation Experiment

To save space, we here present only one of the several experiments we performed. In the experiment, the states were

$$\mathbf{q}_1 = (0, 0, 1)^T, \quad \mathbf{q}_2 = (1, 0, 1)^T, \quad \mathbf{q}_3 = (1, 1, 0)^T$$

and the transition probability matrix was

$$\mathbf{A} = \begin{pmatrix} 0.3 & 0.5 & 0.2 \\ 0.2 & 0.4 & 0.4 \\ 0.5 & 0.2 & 0.3 \end{pmatrix}$$

with π = (34/105,\,39/105,\,32/105) $\approx$ (0.3238, 0.3714, 0.3048). The covariances of observation noise $\mathbf{\Sigma}_j$'s were

$$\mathbf{\Sigma}_1 = 0.01\mathbf{I}_3,$$

$$\mathbf{\Sigma}_2 = \begin{pmatrix} 0.01 & 0 & 0 \\ 0 & 0.015 & 0 \\ 0 & 0 & 0.03 \end{pmatrix}$$

$$\mathbf{\Sigma}_3 = \begin{pmatrix} 0.04 & 0.02 & 0.004 \\ 0.02 & 0.17 & -0.02 \\ 0.004 & -0.02 & 0.1 \end{pmatrix}$$

where $\mathbf{I}_3$ denotes the 3×3 identity matrix. We generated a sample state sequence and observation sequence for 1000 time steps.

In the RPCL, we initialized six seed points randomly from the observation space containing the clusters, and $\hat{\Sigma}_j = 0.1\mathbf{I}_3$, $j = 1, \cdots, 6$. We fixed the learning rates at $\alpha_c = 0.001$ and $\alpha_r = 0.0001$.

After scanning the set of observation data points for two times, three seed points diverged far away from the data points while three seed points remained in the clusters. Hence, the determination of k is correct in this experiment.

Using the algorithm in Stage 2, the estimates of the unknown states were found to be

$$\begin{aligned} \hat{\mathbf{q}}_1 &= (-0.0085, -0.0029, 1.0034)^T \\ \hat{\mathbf{q}}_2 &= (0.9989, 0.0081, 0.9934)^T \\ \hat{\mathbf{q}}_3 &= (0.9837, 1.0216, 0.0080)^T \end{aligned}$$

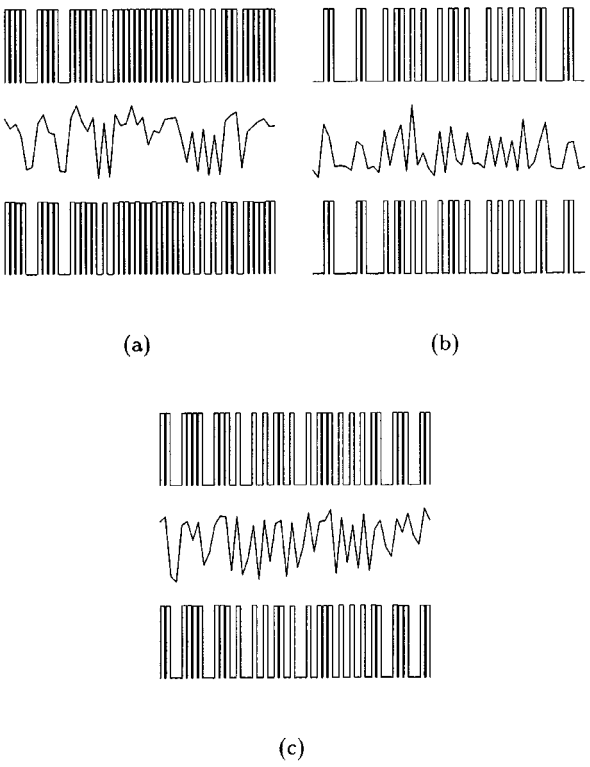

Fig. 2. Slide window showing the original state sequence $\mathbf{s}_t$'s in the first row of (a)–(c), the observations $\mathbf{x}_t$'s in the middle row of (a)–(c), and the recovered state sequence $\hat{\mathbf{s}}_t$'s in the third row of (a)–(c).

whereas the estimates of π, $\{\mathbf{\Sigma}_j\}_{j=1}^k$, and $\mathbf{A}$ were

$$\hat{\pi}_1 = 0.3150, \quad \hat{\pi}_2 = 0.3900, \quad \hat{\pi}_3 = 0.2950,$$

$$\hat{\mathbf{\Sigma}}_1 = \begin{pmatrix} 0.0122 & 0.0005 & -0.0001 \\ 0.0005 & 0.0099 & -0.0001 \\ -0.0001 & -0.0001 & 0.0094 \end{pmatrix}$$

$$\hat{\mathbf{\Sigma}}_2 = \begin{pmatrix} 0.0093 & 0.0000 & 0.0010 \\ 0.0000 & 0.0151 & -0.0001 \\ 0.0010 & -0.0001 & 0.0274 \end{pmatrix}$$

$$\hat{\mathbf{\Sigma}}_3 = \begin{pmatrix} 0.0415 & 0.0153 & 0.0056 \\ 0.0153 & 0.1560 & -0.0262 \\ 0.0056 & -0.0262 & 0.0954 \end{pmatrix}$$

$$\hat{\mathbf{A}} = \begin{pmatrix} 0.3397 & 0.4889 & 0.1714 \\ 0.1620 & 0.4344 & 0.4036 \\ 0.4881 & 0.2271 & 0.2847 \end{pmatrix}.$$

Fig. 2 shows a slide window of the original state sequence, observations, and the estimated state sequence. As we can see, the original state sequence has been almost totally recovered with few state-level errors.

VI. Concluding Remarks

In this paper, we have presented a RPCL-based identification approach for the multidimensional-state Markov model with clustering property. The experiment shows that this approach can successfully identify the model with the correct number of states decided automatically. When the algorithm presented is in batch way, adaptive variants can be made and further studied.

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