Learning Hidden Markov Models using Non-Negative Matrix Factorization

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Abstract—The Baum-Welch algorithm together with its derivatives and variations has been the main technique for learning Hidden Markov Models (HMM) from observational data. We present an HMM learning algorithm based on the non-negative matrix factorization (NMF) of higher order Markovian statistics that is structurally different from the Baum-Welch and its associated approaches. The described algorithm supports estimation of the number of recurrent states of an HMM and iterates the non-negative matrix factorization (NMF) algorithm to improve the learned HMM parameters. Numerical examples are provided as well.

Index Terms—Hidden Markov Models, machine learning, non-negative matrix factorization.

I. INTRODUCTION

Hidden Markov Models (HMM) have been successfully used to model stochastic systems arising in a variety of applications ranging from biology to engineering to finance [1], [2], [3], [4], [5], [6]. Following accepted notation for representing the parameters and structure of HMM's (see [7], [8], [9], [1], [10] for example), we will use the following terminology and definitions:

- 1) N is the number of states of the Markov chain underlying the HMM. The state space is $S = \{S_1, ..., S_N\}$ and the system's state process at time t is denoted by x_t ;
- 2) M is the number of distinct observables or symbols generated by the HMM. The set of possible observables is $\mathcal{V} = \{v_1, ..., v_M\}$ and the observation process at time t is denoted by y_t . We denote by $y_{t_1}^{t_2}$ the subprocess $y_{t_1}y_{t_1+1}...y_{t_2}$;
- 3) The joint probabilities

$$a_{ij}(k) = P(x_{t+1} = S_j, y_{t+1} = v_k | x_t = S_i);$$

are the time-invariant probabilities of transitioning to state S_j at time t+1 and emitting observation v_k given that at time t the system was in state S_i . Observation v_k is emitted during the transition from state S_i to state S_j . We use $A(k) = (a_{ij}(k))$ to denote the matrix of state transition probabilities that emit the same symbol v_k . Note that $A = \sum_k A(k)$ is the stochastic matrix representing the Markov chain state process x_t .

4) The initial state distribution, at time t=1, is given by $\Gamma=\{\gamma_1,...,\gamma_N\}$ where $\gamma_i=P(x_1=S_i)\geq 0$ and $\sum_i \gamma_i=1$.

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V. Crespi is with the Department of Computer Science, California State University at Los Angeles, LA, 90032 USA e-mail: vcrespi@calstatela.edu. Manuscript submitted September 2008 Collectively, matrices A(k) and Γ completely define the HMM and we say that a model for the HMM is $\lambda = (\{A(k) \mid 1 \le k \le M\}, \Gamma)$.

We present an algorithm for *learning* an HMM from single or multiple observation sequences. The traditional approach for learning an HMM is the Baum-Welch Algorithm [1] which has been extended in a variety of ways by others [11], [12], [13].

Recently, a novel and promising approach to the HMM approximation problem was proposed by Finesso et al. [14]. That approach is based on Anderson's HMM stochastic realization technique [15] which demonstrates that a positive factorization of a certain Hankel matrix (consisting of observation string probabilities) can be used to recover the hidden Markov model's probability matrices. Finesso and his coauthors used recently developed non-negative matrix factorization (NMF) algorithms [16] to express those stochastic realization techniques as an operational algorithm. Earlier ideas in that vein were anticipated by Upper in 1997 [17], although that work did not benefit from HMM stochastic realization techniques or NMF algorithms, both of which were developed after 1997.

Methods based on stochastic realization techniques, including the one presented here, are fundamentally different from Baum-Welch based methods in that the algorithms use as input observation sequence *probabilities* as opposed to raw observation *sequences*. Anderson's and Finesso's approaches use system realization methods while our algorithm is in the spirit of the Myhill-Nerode [18] construction for building automata from languages. In the Myhill-Nerode construction, states are defined as equivalence classes of pasts which produce the same futures. In an HMM, the "future" of a state is a probability distribution over future observations. Following this intuition we derive our result in a manner that appears comparatively more concise and elementary, in relation to the aforementioned approaches by Anderson and Finesso.

At a conceptual level, our algorithm operates as follows. We first estimate the matrix of an observation sequence's high order statistics. This matrix has a natural non-negative matrix factorization (NMF) [16] which can be interpreted in terms of the probability distribution of future observations given the current state of the underlying Markov Chain. Once estimated, these probability distributions can be used to directly estimate the transition probabilities of the HMM.

The estimated HMM parameters can be used, in turn, to compute the NMF matrix factors as well as the underlying higher order correlation matrix from data generated by the estimated HMM. We present a simple example in which an NMF factorization is exact but does not correspond to any

HMM. This is a fact that can be established by comparing the factors computed by the NMF with the factors computed by the estimated HMM parameters. This kind of comparison is not possible with other approaches [14].

It is important to point out that the optimal non-negative matrix factorization of a positive matrix is known to be NP-Hard in the general case [19], so in practice one computes only locally optimal factorizations. As we will show through examples, the repeated iteration of the factorization and transition probability estimation steps improves the factorizations and overall model estimation. Details are provided below.

A. Preliminaries and Notation

The only input to our algorithm is an observation sequence of length T of the HMM, namely:

$$\mathcal{O}_{1:T} = \mathcal{O}_1 \mathcal{O}_2 ... \mathcal{O}_T$$

where $\mathcal{O}_t \in \mathcal{V}$ is the HMM output at observation time t.

We do not assume that the observation time t=1 coincides with the process' initial state so that the initial distribution of states is not necessarily governed by Γ . In fact, at present, our algorithm is capable of learning only the ergodic partition of an HMM, namely the set of states that are recurrent. Consequently, our model of an HMM refers only to the transition probability component $\lambda = \{A(k)\}_k$ that identifies this ergodic partition (see [20], [21] for some background on this concept).

Given $\mathcal{O}_{1:T}$, we construct two summary statistics represented as matrices $R^{p,s}$ and $F^{p,s}$ for positive integers p and s. $R^{p,s}$ is simply a histogram of contiguous prefix-suffix combinations whose rows are indexed by observations subsequences of length p and columns are indexed by observation subsequences of length s.

If there are M symbols in the observation alphabet, then $R^{p,s}$ is an M^p by M^s matrix whose (i,j)th entry is the number of times the prefix substring corresponding to i is immediately followed by the substring corresponding to j. The correspondence between strings and integers is lexicographic in our examples below although any other correspondence will do as well.

The matrix $F^{p,s}$ is simply $R^{p,s}$ normalized to be row stochastic. Specifically, if $G=(g_i)$ where $g_i=\sum_j R_{i,j}^{p,s}$ then $F_{i,j}^{p,s}=R_{i,j}^{p,s}/g_i$ for $g_i\neq 0$ and $F_{i,j}^{p,s}=0$ for $g_i=0$. Rows of $R^{p,s}$, and correspondingly $F^{p,s}$, are zero if the prefix corresponding to the row label is not observed in the data. Zero rows of these matrices can be deleted reducing the size of the matrices without affecting the algorithm describe below. Accordingly, $F^{p,s}$ is constructed to be row stochastic.

Entry $F_{u,v}^{p,s}$ is essentially an estimate of P(V|U) the probability of observing observation sequence V of length s, indexed by v, following observation sequence U of length p, indexed by u (see the work of Marton, Katalin and Shields [22] for a study of the accuracy of such estimates).

Note that while R, F and G have exponentially many rows and columns with respect to p and s, the actual number of nonzero entries in these matrices are bounded above by T so that, stored as sparse matrices, they require no more storage

than the original observation sequence. Note that Baum-Welch methods require storing and repeatedly accessing the original observation sequence.

A simple but key observation about states of an HMM is that each state of an HMM induces a probability distribution on symbol subsequences of any length s. Specifically, suppose an HMM, λ , is in state S_{i_0} (having not yet emitted an observation in that state) and consider the symbol subsequence $V = v_{i_1}v_{i_2}...v_{i_s}$. Then

$$P(V|S_{i_0}, s, \lambda) = P(y_{t+1}^{t+s} = v_{j_1}v_{j_2}...v_{j_s}|x_t = S_{i_0})$$

is independent of t under the ergodic assumption and can be computed from the A(k)'s according to

$$P(V|S_{i_0}, s, \lambda) = e'_{S_{i_0}} \prod_{r=1}^{s} A(j_r) \mathbf{1} , \qquad (1)$$

where e_i denotes the (0,1)-vector whose only nonzero entry is in position i and $\mathbf{1} = [1 \ 1 \ \dots \ 1]'$. Call this probability distribution on substrings of length s, $P(\cdot|S_i,s,\lambda)$. It is known that the distributions $P(\cdot|S_i,s,\lambda)$ for $p+s \ge 2N-1$ are complete characterizations of the ergodic states of the HMM with respect to the observables of the HMM [23], [14].

We now focus attention on substrings that *precede* state occupancy in the HMM's underlying Markov chain. Over the course of a long observation sequence such as $\mathcal{O}_{1:T}$, there is some probability, $P(S_i|U,p,\lambda)$ that the HMM is in state i given that we have just observed the length p substring $U=v_{j_1}v_{j_2}\ldots v_{j_p}$. These probabilities can be computed from the A(k)'s according to

$$P(S_{i_0}|U, p, \lambda) = \frac{\pi' \prod_{r=1}^{p} A(j_r) e_{s_{i_0}}}{P(U|p, \lambda)} , \qquad (2)$$

where π is the stationary distribution of the underlying Markov chain process and $P(U|p,\lambda) = \pi' \prod_{r=1}^p A(j_r) \mathbf{1}$.

Note that formulas (1) and (2) are closely related to computations arising in the classical Viterbi algorithm [1].

Let U, V be two strings of observations of length p and s respectively. Let U and V be identified with integers u and v as already explained before so that $P(V|U,\lambda) = F_{u,v}^{p,s}$. Assume V was emitted after time t and U immediately preceded V. We call U the prefix string and V the suffix string. Then by applying elementary properties of probability we can write:

$$F_{u,v}^{p,s} \sim P(y_{t+1}^{t+s} = V \mid y_{t-p+1}^{t} = U, \lambda)$$

$$= \sum_{k=1}^{N} P(y_{t+1}^{t+s} = V, x_{t} = S_{k} | y_{t-p+1}^{t} = U, \lambda)$$

$$= \sum_{k=1}^{N} P(V | S_{k}, s, \lambda) P(S_{k} | U, p, \lambda) .$$

Consequently we can express the distribution $F_{u,:}^{p,s} \sim P(\cdot|U,\lambda)$ as a mixture

$$F_{u,:}^{p,s} \sim \sum_{k=1}^{N} P(\cdot|S_k, s, \lambda) P(S_k|U, p, \lambda) . \tag{3}$$

If the underlying state process x_t is ergodic then in the limit as $T \to \infty$ relation (3) becomes an equality *almost surely*. As

a result of the above observations, for sufficiently large p and s, the matrix $F^{p,s}$ has the following properties:

- $\operatorname{rank}(F^{p,s}) \leq N$, where N is the minimal number of states representing the HMM, λ ;
- Each row of $F^{p,s}$ is a convex combination (mixture) of the N generators, $P(\cdot|S_i,s,\lambda)$, for $i=1,2,\ldots,N$.;
- Letting D be the $N \times M^s$ nonnegative matrix whose rows are the distributions $P(\cdot|S_k,s,\lambda)$, i.e., $D_{k,:}=P(\cdot|S_k,s,\lambda)$, for $k=1,2,\ldots,N$, we can rewrite (3) as

$$F_{u}^{p,s} \sim [P(S_1|U,p,\lambda) \ P(S_2|U,p,\lambda) \ \cdots \ P(S_N|U,p,\lambda)] *D$$

Consequently, if we let $C=(c_{u,k})$ be the $M^p\times N$ nonnegative matrix with $c_{u,k}=P(S_k|U,p,\lambda)$ we can write $F^{p,s}\sim C*D$. Observe that C and D are both (row) stochastic.

The factorization depends on the model λ . Moreover factors C and D can be computed directly from λ using (1) and (2). Consequently, the size of the smallest model compatible with the data is equal to $prank(F^{p,s})$, the positive rank of $F^{p,s}$. (The positive rank, prank(A), of an $m \times n$ nonnegative matrix A is the smallest integer N such that A factors in the product of two nonnegative matrices of dimensions $m \times N$ and $N \times n$ respectively.) It is known that $rank(A) \leq prank(A) \leq$ $\min\{m,n\}$ and that the computation of prank(A) is NP-hard [19], [24]. So it would appear that in general it is NP-hard to estimate N given $F^{p,s}$ even in ideal conditions $(T \to \infty)$ since $\operatorname{rank}(F^{p,s}) \leq N$. However, it is not obvious how difficult it is to estimate when $\operatorname{prank}(F^{p,s}) < \operatorname{rank}(F^{p,s})$ in the case $F^{p,s}$ was built from a typical realization of an HMM. In fact, typically rank($[P(V|U)]_{U,V}$) \leq rank($P(V|S)_{S,V}$) \leq $\operatorname{prank}([P(V|U)]_{U,V})$ but, in "noisy" conditions, we observe $\operatorname{rank}(D) \leq \operatorname{prank}(F^{p,s}) < \operatorname{rank}(F^{p,s})$. We discuss an example at the end of this paper that illustrates the open problems and challenges. One way to circumvent the problem of guessing N is to apply statistical methods directly to the observation sequence, without building any intermediate models as done in [25].

To summarize this discussion, note that the matrix $F^{p,s}$ is based on the distribution of length p prefixes and corresponding length s suffixes and completely characterizes an HMM providing $M^p \geq N, s \geq 2N-1$. Its positive rank is, in ideal conditions, equal to the minimal number of states in the underlying Markov chain. Moreover, an appropriately constructed factorization of $F^{p,s}$ exposes the state transition and emission probabilities of the HMM. It is well known that any two N-state HMMs consistent with the same conditional statistics $[P(V|S)]_{S \in \mathcal{S}, V \in \mathcal{V}^{2N-1}}$ generate the same finite dimensional distributions and so are, in this sense, equivalent [26]. The algorithm presented below extracts the state transition matrices, $\{A(k)\}_k$ from this factorization. In turn, as shown above, the A(k)'s can be used to construct the probability distributions over suffixes that generate $F^{p,s}$ and so can be used to compute a new factorization. This iteration is essentially the basis for our algorithm.

In the machine learning context, we have access only to a finite amount of observation data (T bounded). Consequently rank($F^{p,s}$) will be generally higher than N. This requires a decision about the HMM's order, N, not unlike that arising in principal component analysis (PCA) [27] to estimate the number of components.

II. THE ALGORITHM

Based on the above discussion, our algorithm is outlined below. Numerical examples with discussions follow the formal description.

- 1) Compute $F^{p,s}$ and G from the input observation data, $\mathcal{O}_{1:T}$, defined above.
- 2) Estimate the number of states, N, by analyzing the either $F^{p,s}$ or $\mathrm{diag}(G)*F^{p,s}$, both computed in Step 1. In the cases in which $\mathrm{prank}(F^{p,s})=\mathrm{rank}(F^{p,s})$ (e.g. when $\mathrm{rank}(F)\leq 2$) one typical way to obtain this estimate is to compute the SVD (singular value decomposition) of the aforementioned matrices and then observe the rate of decrease of the singular values. For T sufficiently large a significant gap between the N^{th} and the $(N+1)^{\mathrm{th}}$ largest singular value becomes appreciable. Note that since $\mathrm{prank}\geq \mathrm{rank}$, an estimate based on the singular values is a lower bound for the order of the HMM.
- 3) Estimate distributions $P(\cdot|S_i,s,\lambda)$, for $i=1,2,\ldots,N$. This step is achieved through the Nonnegative Matrix Factorization (NMF) of $F^{p,s}$. This yields $F^{p,s} \approx C*D$ with $D_{i,:} \approx P(\cdot|S_i,s,\lambda)$ as observed before. Note that because of the finiteness of T in general prank $(F^{p,s}) > N$. So it is necessary to solve the approximate NMF which consists of determining C and D of dimensions $M^p \times N$ and $N \times M^s$ respectively that minimize $D_{ID}(F^{p,s}||C*D)$, where

$$D_{ID}(K||W) = \sum_{ij} (K_{ij} \log \frac{K_{ij}}{W_{ij}} - K_{ij} + W_{ij})$$

is the I-divergence function [7] (observe that if $\mathbf{1}'K\mathbf{1} = \mathbf{1}'W\mathbf{1} = 1$ then $D_{ID}(K||W) = \sum_{i,j} K_{i,j} \log K_{i,j}/W_{i,j}$ so the I-divergence function is a generalization of the Kullback-Leibler distance between probability distributions). This optimization problem can be solved through iterative methods [16], [28] that require initial matrices C_0 , D_0 and can only be guaranteed to converge to local optima. After executing this step, we have a locally optimal estimate of the true distributions $P(\cdot|S_i,s,\lambda)$.

4) Estimate matrices A(k), $k=1,2,\ldots,N$, from D. Let us consider $A(1)=(a_{i,j}(1))$, the other matrices are estimated in a similar manner. Let $V^{(s-1)}=v_{j_1}v_{j_2}\cdots v_{j_{s-1}}$ be a generic sequence of s-1 observations. Then by marginalization we can write

$$P(V^{(s-1)}|S_i, s-1, \lambda) = \sum_{k=1}^{M} P(V^{(s-1)}v_k|S_i, s, \lambda) .$$

Consequently, the conditional distributions over suffixes of length s-1, $P(\cdot|S_i,s-1,\lambda)$, can be estimated from D by adding columns of D appropriately. Let

H be the matrix thus obtained from D so that $H_{i,:} \approx$ $P(\cdot|S_i, s-1, \lambda)$. Those conditional distributions satisfy the following equality for any $V^{(s-1)}$:

$$P(v_1V^{(s-1)}|S_i, s, \lambda) = \sum_{j=1}^{N} a_{i,j}(1)P(V^{(s-1)}|S_j, s-1, \lambda).$$

Therefore $P(v_1 \cdot | S_i, s, \lambda) = \sum_{j=1}^N a_{i,j}(1)P(\cdot | S_j, s - s)$ $(1,\lambda)$ so we can obtain the unknown values $a_{i,j}(1)$ by solving the following systems of linear equations:

$$D_{i,1:M^{s-1}} = A_{i,:}(1) * H, i = 1, 2, ..., N$$

where $A_{i,:}(1) = [a_{i,1}(1) \ a_{i,2}(1) \cdots a_{i,N}(1)]$. Compactly $D_{:,1:M^{s-1}} = A(1) * H$. As in step 2, because of the finiteness of T and working with bounded arithmetic precision we need to content ourselves with a solution that minimizes some distance (for example, the L_1 norm) between $D_{i,1:M^{s-1}}$ and $A_{i,i}(1)*H$, for all i. We have formulated these problems as linear programming problems using the L_1 norm.

- 5) Output estimated HMM $\lambda' = \{A(k) \mid k = 1, 2, \dots, N\}.$ This algorithm can be iterated using the estimated λ' and formula (1) to compute new matrices C'_0 and D'_0 , and then restarting from step 3 above with matrices C_0' and D_0' as initial factors in the approximate NMF. In particular:
 - 6) Compute $D'_0 = [P(j|S_i, s, \lambda')]_{i,j}$ using formula (1).
 - 7) Compute C'₀ by solving the linear programming problem F^{p,s} = C'₀ * D'₀, for a row stochastic C'₀.
 8) Set C₀ := C'₀ and D₀ := D'₀.

Another possibility for step 7) above is to compute C'_0 using formulae (2) and (3) and then use the resulting C'_0 and D_0' as initial guesses for the NMF algorithm. We have tried this variant but it does not produce significantly different final results.

III. NUMERICAL EXAMPLES

We call an HMM "Deterministic" (DHMM) if for each state there exists at most one outgoing transition labeled with the same observable. We demonstrate our method on a DHMM, on an HMM that can be transformed into an equivalent DHMM and also on an HMM for which such a transformation does not exist. We finally discuss an example that illustrates the situation when rank < prank.

It is important to note that the significant metric for learning an HMM is *not* the extent to which the transition probabilities are accurately learned but the extent to which the observation statistics are learned. This is a consequence of the fact that HMM's with different transition probabilities and different numbers of states can produce observations sequences with the same statistics so that learning a specific transition probability characterization is not a well-posed problem unless additional constraints to the learning problem are imposed [29].

In our examples we measure the accuracy of our estimates by computing the I-divergence rate of the finite dimensional distributions associated with the observation process of the original model from those associated with the observation process of the estimated model. Formally, each HMM λ induces a family of finite dimensional distributions

$$P_n(y_1^n) = \sum_{i=1}^{N} \pi_i P(y_1^n | x_1 = S_i, \lambda)$$

on sequences of observations of length n, where π is the stationary distribution of the underlying state process. Let λ and λ' be two HMM's with P_n and Q_n their respective induced finite dimensional distributions. The I-divergence rate of λ from λ' is defined as

$$\overline{D}_{ID} = \lim_{n \to \infty} \frac{1}{n} D_{ID}(P_n || Q_n)$$

when the limit exists [14]

A. A DHMM Example

Consider the stochastic process described by model λ_1 = $(\{A(0), A(1)\}, \Gamma = [0 \ 1])$ with

$$A(0)=\left[egin{array}{cc} 0.5 & 0 \\ 0 & 0 \end{array}
ight] \qquad {
m and} \qquad A(1)=\left[egin{array}{cc} 0 & 0.5 \\ 1 & 0 \end{array}
ight] \; .$$

This is sometimes referred to as the "Even Process" [30], [31]. We simulated this process and produced a sequence of T=1000 observations. Then we ran our algorithm with p=2 and

1) Build $F^{2,3}$ from data \mathcal{O} :

$$F = \left[\begin{array}{ccccccccc} 0.14 & 0.13 & 0 & 0.26 & 0 & 0 & 0.22 & 0.26 \\ 0 & 0 & 0 & 0 & 0.25 & 0.24 & 0 & 0.5 \\ 0.13 & 0.14 & 0 & 0.23 & 0 & 0 & 0.26 & 0.24 \\ 0.08 & 0.07 & 0 & 0.17 & 0.08 & 0.08 & 0.17 & 0.33 \end{array} \right]$$

2) Estimate $N = \operatorname{prank}(F)$. Analyze singular values of F:

$$[0.88 \quad 0.48 \quad 0.033 \quad 0.011]$$
.

This suggests rank(F) = prank(F) = 2.

3) Estimate distributions $P(\cdot|S_1,3,\lambda_1)$ and $P(\cdot|S_2,3,\lambda_1)$ by solving $\operatorname{arg\,min}_{C,D} D_{ID}(F||C*D)$:

$$C = \left[\begin{array}{ccc} 0.02 & 0.98 \\ 1 & 0 \\ 0 & 1 \\ 0.34 & 0.66 \end{array} \right] ,$$

$$D = \left[\begin{array}{cccccc} 0 & 0 & 0 & 0.0 & 0.25 & 0.24 & 0.0 & 0.5 \\ 0.13 & 0.13 & 0 & 0.25 & 0 & 0 & 0.25 & 0.24 \end{array} \right]$$

4) Estimate matrices A(0) and A(1):

$$\tilde{A}(0) = \left[\begin{array}{cc} 2.2e - 18 & 0 \\ 6.9e - 18 & 0.51 \end{array} \right], \\ \tilde{A}(1) = \left[\begin{array}{cc} 0.0077 & 0.99 \\ 0.49 & 0 \end{array} \right] \; .$$

After a second iteration of the algorithm the reconstructed matrices become:

$$\hat{A}(0) = \begin{bmatrix} 0 & 0 \\ 5.6e - 17 & 0.51 \end{bmatrix} \hat{A}(1) = \begin{bmatrix} 0.0077 & 0.99 \\ 0.49 & 0 \end{bmatrix}.$$

The reconstructed model is essentially identical to the original one except for state reordering. This result is competitive with existing techniques specific for the machine learning of DHMMs. For example, Shalizi et al [32], [30] demonstrated their Causal-State Splitting Reconstruction (CSSR) ϵ -machine reconstruction algorithm on the same Even Process obtaining comparably accurate models.

B. An HMM that has an equivalent DHMM

Consider the model $\lambda_2 = (\{A(0), A(1)\}, \Gamma = [0\ 1])$ with

$$A(0) = \left[\begin{array}{cc} 0.67 & 0.33 \\ 0 & 0 \end{array} \right] \quad \text{ and } \quad A(1) = \left[\begin{array}{cc} 0 & 0 \\ 1 & 0 \end{array} \right] \; .$$

We simulated this process and produced a sequence of T=10000 observations. Then we ran our algorithm with p=2 and s=3:

1) Build $F^{2,3}$ from data \mathcal{O} :

2) Estimate N. Analyze singular values of F:

$$\begin{bmatrix} 0.86 & 0.24 & 0.02 & 0 \end{bmatrix}$$

to estimate N. This suggests again N=2.

3) Estimate distributions $P(\cdot|S_1,3,\lambda_2)$ and $P(\cdot|S_2,3,\lambda_2)$. Solve $\arg\min_{C,D} D_{ID}(F||C*D)$:

$$C = \left[\begin{array}{cc} 0 & 1 \\ 1 & 0 \\ 0 & 1 \\ 0 & 0 \end{array} \right] ,$$

$$D = \left[\begin{array}{cccccc} 0.44 & 0.23 & 0.33 & 0 & 0 & 0 & 0 & 0 \\ 0.30 & 0.15 & 0.22 & 0 & 0.22 & 0.11 & 0 & 0 \end{array} \right]$$

4) Reconstruct matrices $\tilde{\lambda}_2 = {\tilde{A}(0), \tilde{A}(1)}$:

$$\tilde{A}(0) = \left[\begin{array}{cc} 0.0033 & 0.9967 \\ 0 & 0.6691 \end{array} \right], \\ \tilde{A}(1) = \left[\begin{array}{cc} 0 & 0 \\ 0.3309 & 0 \end{array} \right] \; .$$

After a second iteration of the algorithm the reconstructed model becomes $\hat{\lambda}_2 = \{\hat{A}(0), \hat{A}(1)\}$:

$$\hat{A}(0) = \left[\begin{array}{cc} 0.0039 & 0.996 \\ 0 & 0.6689 \end{array} \right], \hat{A}(1) = \left[\begin{array}{cc} 0 & 0 \\ 0.3311 & 0 \end{array} \right] \ .$$

These computed transition probabilities are different enough from the transition probabilities of the original HMM used to generate the data but the statistics of the observation sequences are very close. Figure 1 shows the accuracy of these estimates in terms of the I-divergence rate of the original model from the estimated ones. We computed $D_{ID}(P_n||Q_n)/n$ for $n=1,2,\ldots,15$, with P_n being the finite dimensional probability distributions over sequences of observations of length n emitted by model λ_2 and Q_n those emitted by the estimates $\tilde{\lambda}_2$ and $\hat{\lambda}_2$, in stationary conditions (the dotted curve refers to $\tilde{\lambda}_2$). We can observe that this quantity, the divergence rate of P_n from Q_n , stabilizes to a very small value (smaller than $2.5 \cdot 10^{-5}$) as expected.

In fact, this example is equivalent to a DHMM model as the reader can readily check independently.

C. An HMM that has no equivalent finite state DHMM

Consider the model $\lambda_3 = (\{A(0), A(1)\}, \Gamma = [1 \ 0 \ 0])$ with

$$A(0) = \begin{bmatrix} 0.5 & 0.5 & 0 \\ 0 & 0.5 & 0 \\ 0.5 & 0.5 & 0 \end{bmatrix} \quad \text{ and } \quad A(1) = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0.5 \\ 0 & 0 & 0 \end{bmatrix}.$$

We simulated this process and produced a sequence of T=10000 observations. Then we ran our algorithm with p=4 and s=5. After the first iteration we obtain $\tilde{\lambda}_3$:

$$\tilde{A}(0) = \begin{bmatrix} 0 & 0.2 & 0.8 \\ 0 & 0.35 & 0 \\ 0 & 0.4 & 0.6 \end{bmatrix}, \tilde{A}(1) = \begin{bmatrix} 0 & 0 & 0 \\ 0.1 & 0 & 0.56 \\ 0 & 0 & 0 \end{bmatrix}.$$

After the second iteration we obtain $\hat{\lambda}_3$:

$$\hat{A}(0) = \begin{bmatrix} 0 & 0.2 & 0.8 \\ 0 & 0.36 & 0 \\ 0 & 0.41 & 0.59 \end{bmatrix}, \hat{A}(1) = \begin{bmatrix} 0 & 0 & 0 \\ 0.09 & 0 & 0.56 \\ 0 & 0 & 0 \end{bmatrix}.$$

As before, Figure 1 (bottom) shows the accuracy of these estimates in terms of the I-divergence rate of the original model from the estimated ones.

Observe that this HMM cannot be transformed into an equivalent deterministic HMM [33].

D. Discussion of Rank vs Prank

We first provide an example of a stochastic matrix whose prank differs from its rank but that matrix does not represent the statistics of any HMM.

$$F = \frac{1}{16} \cdot \begin{bmatrix} 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 1 \end{bmatrix} \otimes \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 \end{bmatrix},$$

where \otimes is the Kronecker product. We can verify that $\operatorname{rank}(F) = 3$ whereas $\operatorname{prank}(F) = 4$ [28]. Moreover F = CD exactly with

$$C = \begin{bmatrix} 0.5 & 0 & 0.5 & 0 \\ 0.5 & 0.5 & 0 & 0 \\ 0 & 0 & 0.5 & 0.5 \\ 0 & 0.5 & 0 & 0.5 \end{bmatrix}$$

and

$$D = \frac{1}{8} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \otimes \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 \end{bmatrix}.$$

Assume that F was obtained from a typical sequence of observations emitted by an HMM λ with 4 states so that $F^{2,5} = F = CD$. Then it must be that $C = [P(S_j|i,2,\lambda)]_{i,j}$ and $D = [P(k|S_j,5,\lambda)]_{j,k}$. Consider the following model $\lambda = \{A(1),A(2)\}$ with

$$A(0) = \left[\begin{array}{cccc} 0.5 & 0 & 0.5 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0.5 & 0 & 0.5 \\ 0 & 0 & 0 & 0 \end{array} \right], A(1) = \left[\begin{array}{cccc} 0 & 0 & 0 & 0 \\ 0.5 & 0 & 0.5 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0.5 & 0 & 0.5 \end{array} \right].$$

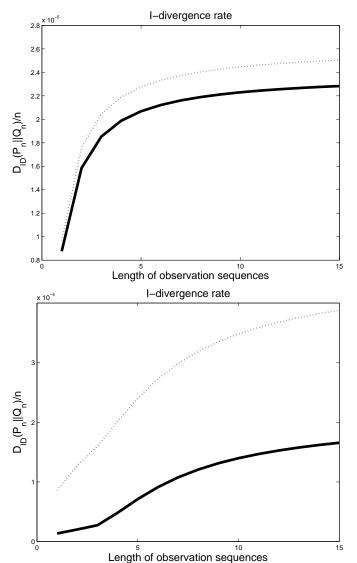


Fig. 1. Accuracy of HMM's $\tilde{\lambda}_2$, $\hat{\lambda}_2$ (top) and $\tilde{\lambda}_3$, $\hat{\lambda}_3$ (bottom). Here P_n is the distribution over sequences of observations of fixed length n induced by the original model whereas Q_n refers to the estimated models. The sequence $D_{ID}(P_n||Q_n)/n$ is calculated for increasing values of n. The dotted curves refer to $\tilde{\lambda}_2$ (top) and $\tilde{\lambda}_3$ (bottom).

One can verify that λ is the only four-state model such that $D = [P(k|S_j, 5, \lambda)]_{j,k}$. In fact observe that the system of equations defining λ in stage 4 of the algorithm admits, in this case, only one solution. Nevertheless, using formula (2):

$$[P(S_j|i,2,\lambda)]_{i,j} = (1/4) * \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} \otimes \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} \neq C.$$

Consequently no HMM can generate F.

1) An example of prank > rank for an exact HMM model: The following four-state model λ is an example of an HMM whose induced $F^{2,5}$ matrix has rank 3 but positive rank prank = 4:

To verify the claim we computed factors $C = [P(S_j|i,\lambda)]_{i,j}$ and $D = [P(j|S_i,5,\lambda)]_{i,j}$, for N=4, using formulae (1) and (2) and then obtained $F^{2,5} = C*D$. Then we verified numerically that $\mathrm{rank}(F^{2,5}) = 3$. Finally, we applied Lemma 2.4 in [28] to confirm that $\mathrm{prank}(F^{2,5}) = 4$. We also verified the character of this model by directly applying our algorithm to it in order to obtain $F^{2,5}$ empirically (for T=10000). An analysis of the singular values of $F^{2,5}$, namely $[0.8530\ 0.4825\ 0.1799\ 0.0114]$, demonstrates the difficulty of this case. The fourth singular value is nonzero due to the finiteness of T. Consequently it is difficult to determine whether N=3 or N=4.

IV. OPEN QUESTIONS AND FUTURE WORK

A crucial issue is the estimation of N, the size of the smallest HMM that generates the stream of data. Under ideal conditions, $(T \to \infty)$, we have seen that $N = \operatorname{prank}(F^{p,s})$. However, filtering out "noise" from the empirical matrix $F^{p,s}$ in order to have an accurate estimate of the positive rank is an open challenge. Observe that a spectral analysis of F may, in general, produce only a lower bound to N.

A second important issue in our methodology concerns the computation of the approximate NMF. Existing methods are suboptimal due to the presence of local optima. This problem affects the accuracy of the produced estimate at each iteration of our algorithm. Consequently it is important to investigate convergence properties when stages 3-5 of the algorithm are iterated with new initial factors C_0' , D_0' to seed the approximate NMF, using C_0' and D_0' as computed according to steps 6-8, from model λ' that was estimated in the preceding step.

A third question concerns with properties of $F^{p,s}$ as $s \to \infty$. In other words, can the Asymptotic Equipartition Property be applied to distributions $P(\cdot|S_i,s,\lambda)$ so that the distribution on the "typical" finite suffixes is uniform and the rest of the distribution is zero?

V. CONCLUSION

We have presented a new algorithm for learning an HMM from observations of the HMM's output. The algorithm is structurally different from traditional Baum-Welch based approaches [1], [11], [12], [13]. It is related to but different from recent approaches in stochastic systems realization [14]. We believe this method opens a new line of algorithm development for learning HMM's and has the advantage of a estimating the HMM order from spectral properties of the high order correlation statistics of the observation sequence. The algorithm effectively compresses data by summarizing it into a statistical matrix. Options for recursively computing the steps of the algorithm to achieve *on-line* algorithms will be explored. Additionally, sparse matrix algorithms can be explored for space and time efficiency when the underlying matrices are large and sparse.

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