Evaluation of Spectral Learning for the Identification of Hidden Markov Models

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Abstract: Hidden Markov models have successfully been applied as models of discrete time series in many fields. Often, when applied in practice, the parameters of these models have to be estimated. The currently predominating identification methods, such as maximum-likelihood estimation and especially expectation-maximization, are iterative and prone to have problems with local minima. A non-iterative method employing a spectral subspace-like approach has recently been proposed in the machine learning literature. This paper evaluates the performance of this algorithm, and compares it to the performance of the expectation-maximization algorithm, on a number of numerical examples. We find that the performance is mixed; it successfully identifies some systems with relatively few available observations, but fails completely for some systems even when a large amount of observations is available. An open question is how this discrepancy can be explained. We provide some indications that it could be related to how well-conditioned some system parameters are.

Keywords: spectral learning, hidden Markov models, HMM, system identification, spectral factorization, method of moments, performance evaluation

1. INTRODUCTION

Hidden Markov Models (HMMs) are standard tools for modeling discrete time series. They have, among others, been applied to such diverse fields as speech recognition (e.g. Rabiner (1989), Gales and Young (2008)), genomic sequence analysis (e.g. Eddy (1996)) and financial stock prediction (e.g. Hassan and Nath (2005)). The parameters of these models are usually unknown and have to be estimated from data when applied in practice. Methods for performing this task, such as the Expectation-Maximization (EM) algorithm (also referred to as the Baum-Welch algorithm when applied specifically to HMMs), are usually iterative and might encounter problems with local minima and slow convergence (see e.g. Hsu et al. (2012)).

A well-known approach for the identification of linear states-space models is to employ subspace techniques (e.g. Van Overschee and De Moor (1996), or Ljung (1998)). This approach is non-iterative and avoids the concern of local minima that can cause problems when employing EM. There have been attempts to apply similar methods to HMMs (e.g. Vanluyten et al. (2007), Hjalmarsson and Ninness (1998), Anandkumar et al. (2012b), and Hsu et al. (2012)). One of the difficulties with adapting these techniques is that the HMM has some restrictions that are not present for regular linear systems, namely that some parameters represent probabilities and thus have to be non-negative and sum to one.

This paper is concerned with the so-called spectral learning algorithm proposed by Hsu et al. (2012). The idea of their method is to relate observable quantities, correlations in pairs and triplets in a sequence of observations, to the system parameters. The observable quantities are estimated from the available data and used to recover estimates of the parameters of the HMM by reversing the relations. This is fundamentally a method of moments. It has been generalized to other models and put in a tensor decomposition framework in subsequent work, see e.g. Anandkumar et al. (2012a), Anandkumar et al. (2012b), and Anandkumar et al. (2014).

The contribution of this paper is an evaluation of how the spectral learning algorithm performs on a number of systems. We find that its performance is varied. It identifies some systems well using a small amount of observations, but fails to identify some systems even with a large number of observations.

This paper is structured as follows: The HMM is formally introduced in Section 2, along with statistical moments. Section 3 states the identification problem for HMMs. Section 4 outlines the spectral learning algorithm by Hsu et al. (2012). Section 5 discusses how the correctness of the estimates is measured. Section 6 provides numerical results from simulations for SL and EM. Section 7 concludes the paper with a brief discussion of the results.

* This work was partially supported by the Swedish Research Council and the Linnaeus Center ACCESS at KTH. The research leading to these results has received funding from The European Research Council under the European Community’s Seventh Framework program (FP7 2007-2013) / ERC Grant Agreement N. 267381.
2. PRELIMINARIES

Vectors in this paper are assumed to be column vectors and we use the symbol $\hat{\cdot}$ to denote an empirical estimate of a numerical quantity.

2.1 Hidden Markov Models

The HMM is a generalization of the Markov chain, which is a discrete stochastic model that can be represented as a sequence of stochastic variables, say $x_1, x_2, \ldots$. These variables take values in some set $X = \{1, 2, \ldots, X\}$, which is called the state-space (of dimension $X \in \mathbb{N}^+$). The crucial assumption of a Markov chain is that the Markov state of the Markov chain is not directly observed and we use the symbol $\pi_i$ to refer to the $i$th canonical (column) unit vector. Details to handle the case that $Y > X$ can be found in e.g. Hsu et al. (2012), Mattila (2015) and Johnson (2012).

The problem we aim to solve is the following: At hand is an HMM-system with unknown parameters. The data that are available is a sequence of consecutive observations $y_1, y_2, \ldots, y_T$. To be able to construct for example an HMM-filter, we want to fit parameters of an HMM such that it models the observed data well. We assume that we know the number of hidden states $X$ and the number of possible observations $Y$ of the true system.

3. PROBLEM FORMULATION

The problem we aim to solve is the following: At hand is an HMM-system with unknown parameters. The data that are available is a sequence of consecutive observations $y_1, y_2, \ldots, y_T$. To be able to construct for example an HMM-filter, we want to fit parameters of an HMM such that it models the observed data well. We assume that we know the number of hidden states $X$ and the number of possible observations $Y$ of the true system.

4. THE SPECTRAL LEARNING ALGORITHM

Hsu et al. (2012) are not mainly concerned with recovering explicit expressions for estimates of the parameters $T, O$ and $\pi_0$, but rather intend to identify another parametrization of the HMM. This parametrization allows them to calculate the probabilities of sequences of observations, for example, the joint distribution $\Pr[y_1, y_2, \ldots, y_k]$ and the conditional distribution $\Pr[y_k+1|y_1, y_2, \ldots, y_k]$. They describe in an appendix how the method by Mossel and Roch (2006) can be used in conjunction with their method to recover explicit expressions for $T, O$ and $\pi_0$. This combined method will be outlined below, and is what we refer to as Spectral Learning (SL).

It is possible to derive the following relations between different moments and the parameters of the HMM:

$$S_1 = O\pi_0,$$
$$S_{2,1} = OT \text{ diag}(\pi_0)OT^T,$$
$$S_{1,1} = OT^2 \text{ diag}(\pi_0)OT^T$$

and

$$S_{3,2,1} = OT \text{ diag}(c_i^T O)T \text{ diag}(\pi_0)OT^T,$$

where $c_i$ is the $i$th canonical (column) unit vector. Details can be found in e.g. Hsu et al. (2012), Mattila (2015) and Johnson (2012).
By employing the relations given above, it can be shown that the same transformation \((U^T O T)^{-1}\) diagonalizes (14) for every \(y\). This is important for preserving the order of the eigenvalues.

The transformation could be recovered for any \(y\), but to increase the robustness of the method, a set of random variables, \(g_y \sim N(0, 1)\) for \(i = 1, 2, \ldots, Y\), is introduced. Here, \(N(\mu, \sigma^2)\) is the normal distribution with mean value \(\mu\) and variance \(\sigma^2\). It can be shown from (14) that

\[
\sum_{y=1}^{Y} g_y (U^T S_{3,y,1}) (U^T S_{3,1})^+ = (U^T O T) \{ \sum_{y=1}^{Y} g_y (e_y^T O) \} (U^T O T)^{-1}
\]

holds.

Thus, by performing an eigendecomposition of the left hand side of (16), we recover the diagonalization transformation \((U^T O T)^{-1}\), up to scaling and permutation of the columns. This matrix is then utilized in (15) to recover each row of \(O\).

\textbf{Remark 1.} If for each \(y\) an eigendecomposition of (14) is performed directly using some numerical method, then the elements of \(O\) will be recovered, but since eigenvalues do not have any intrinsic ordering, as \(O\) is assembled (row by row), every row will have its elements sorted according to the order in which the eigenvalues were returned by the method performing the eigendecomposition. Since the columns of \(O\) correspond to the different hidden states of the HMM, a consistent ordering is required. By using the same diagonalization matrix — the one recovered in (16) — we guarantee that the eigenvalues have a consistent ordering.

Once \(O\) is recovered, Hsu et al. (2012) suggest that the following expressions be used to recover the other parameters:

\[
\pi_0 = O^+ S_1
\]

and

\[
T = O^+ S_{2,1} (O^+)^T \text{diag}(\pi_0)^{-1}.
\]

**Algorithm 1** Spectral Learning from Hsu et al. (2012)

1. Sample triplets of observations \((y_1, y_2, y_3)\) from the HMM and form empirical estimates \(S_1, \hat{S}_{2,1}, \hat{S}_{3,1}\) and \(\hat{S}_{3,2,1}\) for \(y = 1, \ldots, Y\).
2. Calculate the SVD of \(\hat{S}_{2,1}\) and form \(\hat{U}\) by taking the left singular vectors corresponding to the \(X\) largest singular values as columns.
3. Generate \(Y\) normally distributed random variables \(g_y \sim N(0, 1)\) for \(y = 1, \ldots, Y\).
4. Perform an eigendecomposition of the left hand side of (16) when the above estimates are used, i.e. of

\[
\sum_{y=1}^{Y} g_y (U^T \hat{S}_{3,y,1}) (U^T \hat{S}_{3,1})^+.
\]

5. Use the matrix of eigenvectors from Step 4 to diagonalize \((U^T \hat{S}_{3,y,1}) (U^T \hat{S}_{3,1})^+\) for \(y = 1, \ldots, Y\) and take the diagonal as row \(y\) of \(\hat{O}\). The diagonalizations are performed by multiplying the left and by the inverse from the right in accordance with (15).
6. Calculate

\[
\hat{\pi} \leftarrow \hat{O}^+ \hat{S}_1
\]

and

\[
\hat{T} \leftarrow \hat{O}^+ \hat{S}_{2,1} (\hat{O}^+)^T \text{diag}(\hat{\pi}_0)^{-1}.
\]

7. Return \(\hat{O}, \hat{T}\) and \(\hat{\pi}_0\).
To employ the method on real data, estimates are to be used for the moments $S_1$, $S_{2,1}$, $S_{3,1}$ and $S_{3,\pi,1}$. This concludes the SL algorithm, which for convenience is summarized in Algorithm 1.

Remark 2. Since in our problem formulation we make the assumption that all our observations are consecutive, unlike Hsu et al. (2012) who independently sample triplets of observations to estimate the different moments, our estimate of the initial distribution will be an estimate of the stationary distribution of the Markov chain corresponding to the transition matrix $T$.

5. ERROR MEASURE

We use the Mean Squared Error (MSE) of the elements in the relevant matrices as a measure of the error of the estimates. For two matrices $A, \hat{A} \in \mathbb{R}^{m \times n}$, the MSE is defined as

$$\text{MSE}(A, \hat{A}) = \|A - \hat{A}\|_F^2,$$

where $\| \cdot \|_F$ denotes the Frobenius norm.

It is important to notice that the columns of $\hat{O}$, and the rows and columns of $\hat{T}$, can be permuted compared to those in $O$ and $T$, depending on the method used to calculate the diagonalization transformation of (16). It is thus not meaningful to calculate and present, for example, $\text{MSE}(O, \hat{O})$ directly.

The columns of $\hat{O}$, and the rows and columns of $\hat{T}$, have to be permuted as to line up with those of the original matrices used to generate the sequence of observations if $\text{MSE}(\cdot, \gamma)$ is to make sense. This is a simple combinatorial problem which is solved in the results to be presented. The intuition behind this is that the order of the hidden states can not be discerned from external observations of the HMM (nor in the case of a regular linear system). It follows from the SL algorithm that HMMs are generically identifiable up to these permutations.

Also notice that there is nothing in SL that enforces the stochasticity constraints on the estimates of $T$, $O$ and $\pi_0$. The elements of $\hat{O}$ are the result of an eigendecomposition, and can therefore turn out to be negative, or even complex. The columns of $\hat{T}$ and $\pi_0$ might also lie outside of $[0,1]$, since they are calculated from $\hat{O}$. This is currently one of the main difficulties of using SL.

6. NUMERICAL RESULTS

This section presents numerical results for SL and EM. All simulations were performed on a 1.3 GHz MacBook Air with 4 GB RAM.

6.1 Spectral Learning

The performance of SL\footnote{The implementation and simulations were performed using MATLAB R2013a.} was evaluated on seven systems (taken from standard texts on HMMs or conceived) and the results are presented in Figures 1 and 2. The systems had three hidden states, and three (Examples 2, 4, 5, 6 and 7) or ten (Examples 3 and 8) possible observations, i.e.

\[X = 3 \text{ and } Y \in \{3, 10\}.\]

The exact numerical parameters (i.e. the transition and observation matrices) for each example can be found in Mattila (2015). Every point in the plots is the average of 20 simulations.

As previously mentioned, there is no guarantee that the estimates recovered by SL are (stochastically) valid. In the rightmost plot of Figure 1, the fraction of these 20 simulations that resulted in estimates with elements with negative or non-zero imaginary components is presented.

SL demonstrated a mixed performance on the examples on which it was evaluated. It converged for a relatively small amount of samples on Examples 3 and 6, but failed to converge even for large amounts of samples for Examples 4, 5 and 8. This can be seen both from the error in the estimates of $T$ and $O$, but also from the fraction of invalid estimates. The performance on Examples 2 and 7 was in between these other two performance classes.

It is worth noting that the slopes of the errors appear to be constant once SL starts providing a large fraction of valid estimates, which happened for different amounts of samples for the different systems.

6.2 Expectation-Maximization Method

For a thorough treatment of the EM-algorithm, see McLachlan and Krishnan (2008). The implementation provided in MATLAB (hmmtrain) was used with the maximum number of iterations taken as the default value of 500. Three of the examples on which SL had varying performance were considered. In Figures 2 and 3, the EM-algorithm was started with random matrices as initial guesses for the HMM parameters.

EM performed better, errorwise, than SL on Examples 2 and 4 when a small amount of observations was available. However, as is apparent in Figure 2, the time-scale is orders of magnitude larger than that of SL. For all of the examples that were considered, when about $10^5$ available samples were available, SL delivered estimates in less than a tenth of a second, whereas EM required about ten minutes.

The initial guesses for the parameters in EM play an important role as can be seen in Figure 3; the error of the estimated $T$ matrix increased for two of the systems as more and more of samples were available. This is probably
due to the random initial guesses being worse in those simulations.

In Figure 4, the true parameters of the HMMs were used as initial guesses in the EM algorithm. To make a comparison between EM and SL easier, we also plot the performance of SL (from Figure 1) as dashed lines in the same figure.

The error for EM when started at the true system parameters is closely related to the Cramér-Rao bounds for how well any estimation method can perform. SL was close to the performance of EM for Example 3, but was far off for the other two examples. Note that the EM curves lie higher for those two examples than for Example 3, implying that the maximum of the likelihood function for the available data lies further away from the true maximum.

6.3 Relation to Condition Numbers

The mixed performance of SL, compared both to EM and to itself on the different examples, could be due to many reasons. One could be that there is a loss of information when only the first, second and third order moments are used, instead of moments up to the length of the whole observation sequence.

Regarding the discrepancy between the different examples, a simple perturbation analysis (Mattila (2015)) shows that the condition number of \((UOT)\) is related to the upper bound on how far the eigenvalues might move in (14) (i.e. the elements of one row of the recovered observation matrix) due to perturbations in the estimates of the moments.

Since the matrix \(U\) in SL is not absolutely specified (the choice as some of the singular vectors is just a suggestion, see Hsu et al. (2012) for details), we provide in Table 1 the condition number of \(OT\) for the different systems in Figure 1. We have sorted the examples after what the MSE was when \(10^7\) samples were available in the estimation procedure. The condition numbers are perfectly sorted except for the outlier Example 8. This suggests that the condition number of \(OT\) could give some indication on how well SL will perform for a given system.

7. CONCLUSION

We have implemented and evaluated the algorithm outlined in Hsu et al. (2012), which uses spectral methods to deliver one-shot estimates of the parameters of an HMM. We saw that the performance of the algorithm is overall good, but that it fails completely for some systems, and that the performance could be related to a certain condition number.

We also observed that SL is orders of magnitude faster than EM, especially when a large amount of observations is available. This suggests that SL could be a preferable alternative to EM in cases where there is a large number of observations available from the HMM. The recovered estimates can then be refined, if necessary, using for example EM. Note that this assumes that the estimates recovered from SL are stochastically valid, which was not the case for many systems. SL started providing valid estimates when different amounts of samples were available for the different systems.

ACKNOWLEDGEMENTS

The authors would like to thank Vikram Krishnamurthy for helpful discussions.

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