EMHMM Simulation Study

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Abstract

Eye Movement analysis with Hidden Markov Models (EMHMM) is a method for modeling
eye fixation sequences using hidden Markov models (HMMs). In this report, we run a
simulation study to investigate the estimation error for learning HMMs with variational
Bayesian inference, with respect to the number of sequences and the sequence lengths. We
also relate the estimation error measured by KL divergence and L1-norm to a corresponding
distortion in the ground-truth HMM parameters.

1. Introduction

Eye Movement analysis with Hidden Markov Models (EMHMM) (Chuk et al., 2014; Chan
and Hsiao, 2017) is a method for modeling eye fixation sequences using hidden Markov
models (HMMs). Given a subject’s eye fixation sequences, a subject’s HMM is learned
using a variational Bayesian approach. In this paper we run a simulation study to investigate
the estimation error for learning HMMs with respect to the number of sequences and the
sequence lengths.

2. Background

We consider an HMM with Gaussian emissions. The joint likelihood of the observation
(fixations) and the hidden state (ROI) sequences is,

$$p(x, z) = p(x|z)p(z) = \prod_{t=2}^{\tau} p(z_t|z_{t-1}) \prod_{t=1}^{\tau} p(x_t|z_t)$$ (1)

where $x = [x_1, \cdots, x_\tau]$ is a sequence of observations and $z = [z_1, \cdots, z_\tau]$ is the sequence of
hidden states, where $x_t \in \mathbb{R}^D$ and $z_t \in \{1, \cdots, K\}$. $D$ is the dimension of the observations,
and $K$ is the number of states. Note that for this simulation study, we assume that the
length of the sequences is the same for all observations.
The observation likelihood, transition probabilities, and initial state probabilities are as follows:

\[
\text{initial state: } \quad p(z_1 = k | \pi) = \pi_k \tag{2}
\]
\[
\text{transition probability: } \quad p(z_t = k | z_{t-1} = j) = a_{j,k} \tag{3}
\]
\[
\text{observation likelihood: } \quad p(x_t | z_t = k) = \mathcal{N}(x_t; \mu_k, \Sigma_k) \tag{4}
\]

where the Gaussian density is

\[
\mathcal{N}(x; \mu, \Sigma) = (2\pi)^{-D/2} |\Sigma|^{-1/2} e^{-\frac{1}{2}(x-\mu)^T \Sigma^{-1} (x-\mu)}, \tag{5}
\]

where \(\Sigma\) is the covariance matrix. The parameters of the HMM are:

- the initial hidden state probabilities: \(\pi = [\pi_1, \cdots, \pi_K]^T\) \(\tag{6}\)
- transition probability \(p(z_t = k | z_{t-1} = j)\): \(a_{j,k}\) \(\tag{7}\)
- transition distribution given \(z_{t-1} = j\): \(a_j = [a_{j,1}, \cdots, a_{j,K}]\) \(\tag{8}\)
- the transition matrix: \(A = [a_{j,k}]_{j,k}\) \(\tag{9}\)
- the mean and covariance matrix for the \(k\)th Gaussian emission: \(\{\mu_k, \Sigma_k\}\) \(\tag{10}\)

The likelihood of an observation sequence \(x\) is obtained by marginalizing out hidden states,

\[
p(x) = \sum_{z} p(x|z)p(z) = \sum_{z_1} \cdots \sum_{z_T} p(x|z)p(z) \tag{11}
\]

The distribution of the initial observation is a Gaussian mixture model (GMM),

\[
p(x_1) = \sum_{j=1}^{K} p(x_1|z_1 = j)p(z_1 = j) = \sum_{j=1}^{K} \pi_j p(x_1|z_1 = j). \tag{12}
\]

### 3. Simulation Procedure

We next outline the simulation procedure for EMHMM. Given a ground-truth HMM, we sample a number of fixation sequences of a given length. Using the sample sequences, we then estimate an HMM using EMHMM, and then compare the estimated HMM with the ground-truth HMM in terms of various metrics.

#### 3.1 Ground-truth HMMs

A ground-truth HMMs \(\Theta\) is created from the fixation sequences collected from a subjects. An HMM was learned from the subject’s data using the EMHMM toolbox, and this HMM is then treated as a ground-truth HMM. The goal then is to estimate another HMM \(\hat{\Theta}\) from the samples generated from the ground-truth HMM \(\Theta\). Note that the “ground-truth HMM” is itself an estimate from a larger collection of data. However, here we are interested in how an HMM estimated from data compares with the original MM used to generate the data, when the number of samples and the sequence lengths vary.
3.2 Estimating HMMs

Given a ground-truth HMM $\Theta$, a set of fixation sequences $\{x^{(n)}\}_{n=1}^N$ are sampled from the HMM according to the probability distribution in (1). Next an HMM $\hat{\Theta}$ is learned from the samples using variational Bayesian estimation, as implemented in EMHMM. The hyperparameters of the model, including the number of states, are estimated automatically by maximizing the marginal likelihood of the data. Hence, it is possible that the predicted number of states $\hat{K}$ is different from the number of states $K$ in the ground-truth HMM.

3.3 Comparing HMMs

The HMM is a probabilistic model for a whole sequence $x$, as in (11). It also contains different distributions, including observation likelihoods, transition probabilities, and initial state probabilities in (2), (3), and (4). Hence, we consider different methods to compare two HMMs, $\Theta$ and $\hat{\Theta}$.

3.3.1 Dissimilarity Measures

We first introduce the two dissimilarity measures that we will use. Consider two probability distributions $p(y)$ and $\hat{p}(y)$, we consider two methods for comparing them.

**Kullback Leibler divergence (KLD):** Kullback Leibler divergence (Kullback, 1997) is a dissimilarity measure between two distributions defined as

$$\phi(p(y), \hat{p}(y)) = \int_y p(y) \log \frac{p(y)}{\hat{p}(y)} \, dy = \mathbb{E}_{y \sim p(y)} \left[ \log \frac{p(y)}{\hat{p}(y)} \right],$$

(13)

The KLD will be 0 when the two distributions are equal to each other, and more positive values indicate more dissimilarity between the two distributions. Intuitively, the KLD is the amount of “information” that needs to be added to turn the approximation $\hat{p}(x)$ into the original $p(x)$. Another interpretation is that the KLD is the weighted average of the log-likelihood ratio between the two models over all sequences, where the weight for each sequence is based on its likelihood of occurring.

In some cases, there is no analytical solution to the integral in (13), and hence we use sampling to approximate the KLD:

$$\phi(p(y), \hat{p}(y)) \approx \frac{1}{S} \sum_{s=1}^{S} \log \frac{p(y^{(s)})}{\hat{p}(y^{(s)})},$$

(14)

where the samples are drawn from $p(y)$, i.e., $y^{(s)} \sim p(y)$.

**L1-norm:** The L1-norm measures the absolute difference between the two distributions,

$$\psi(p(y), \hat{p}(y)) = \frac{1}{2} \int_y |p(y) - \hat{p}(y)| \, dy.$$

(15)

Intuitively, the L1-norm measures the amount of distribution in $\hat{p}(y)$ that needs to be moved to change $\hat{p}(y)$ into $p(y)$. It is also inversely related to the histogram intersection, which
measures the amount of overlapping distribution between \( p(y) \) and \( \hat{p}(y) \),

\[
\int_y \min(p(y), \hat{p}(y)) \, dy = 1 - \psi(p(y), \hat{p}(y))
\]  

When the integral does not have a closed-form solution, then we approximate using numeric integration.

Because it has a more intuitive interpretation related to the percentage of overlap between two probability distributions, we will use L1-norm measurements to compare individual components of the HMM, including the individual ROIs, transition matrices, and initial state probabilities.

3.3.2 Whole HMM

To compare the whole HMMs, we use the Kullback-Leibler divergence rate (Kullback, 1997) between the observation sequence likelihoods in (11). Denote \( p(x) \) and \( \hat{p}(x) \) as the observation sequence likelihood for the ground-truth HMM \( \Theta \) and the estimated HMM \( \hat{\Theta} \). The KLD rate is

\[
D_{HMM} = \frac{1}{T} \phi(p(x), \hat{p}(x)),
\]  

where \( T \) is the sequence length (same as the sequence length of the data).

3.3.3 Matched ROIs

The above comparisons measure differences in the distributions of the whole sequences between two HMMs, considering all ROIs and transitions at the same time. We can also compare the individual ROIs between the two HMMS by matching ROIs between \( \Theta \) and \( \hat{\Theta} \). For now assume that both HMMs have the same number of ROIs. Assuming that the ROI indices already match, the L1-norm between the two HMMs \( \Theta \) and \( \hat{\Theta} \) is

\[
\Psi(\Theta, \hat{\Theta}) = \frac{1}{K} \sum_{j=1}^{K} \psi(p(x_t|z_t = j), \hat{p}(x_t|z_t = j))
\]  

When the ROIs do not match, then we define \( \mathcal{P} \) as the state-permutation operator that permutes (reorders) the states of an HMM, and compute the permutation that minimizes the L1-norm

\[
\ell_{ROI} = \min_{\mathcal{P}} \Psi(\Theta, \mathcal{P}(\hat{\Theta})).
\]  

When the number of ROIs do not match between \( \hat{\Theta} \) and \( \Theta \), e.g., \( \hat{K} < K \), then we duplicate some ROIs in \( \hat{\Theta} \) until \( \hat{K} = K \). In this way, the matching function will match one ROI in \( \hat{\Theta} \) to more than one ROI in \( \Theta \). The ROIs for duplication are selected so as to minimize the final \( \ell_{ROI} \). A similar procedure occurs if \( \hat{K} > K \).
3.3.4 Matched Transition Matrices and Initial States

We directly compare transition matrices and initial state probabilities using a similar matching technique. Here we are interested in whether the underlying state dynamics (transitions and prior) are similar, regardless of the accuracy of the ROIs. For now assume that the number of states is the same in the two HMMs $\Theta$ and $\hat{\Theta}$. Define the L1-norm between two transition matrices,

$$\Psi(A, \hat{A}) = \sum_{i=1}^{K} \sum_{j=1}^{K} |a_{i,j} - \hat{a}_{i,j}|,$$

and the L1-norm between two initial states probability vectors,

$$\Psi(\pi, \hat{\pi}) = \sum_{j=1}^{K} |\pi_j - \hat{\pi}_j|.$$  

We then find the permutation that minimizes the L1-norm between the transition matrices and priors,

$$P^* = \min_{P} \Psi(A, P(\hat{A})) + \Psi(\pi, P(\hat{\pi})).$$  

Given the optimal permutation $P^*$, we compute L1-norms for comparison:

$$\ell_{\text{trans}} = \frac{1}{K} \Psi(A, P^*(\hat{A})),\quad \ell_{\text{prior}} = \Psi(\pi, P^*(\hat{\pi})).$$

When the number of ROIs do not match between $\Theta$ and $\hat{\Theta}$, i.e., $\hat{K} < K$, we augment $\hat{\Theta}$ with enough states to match $\Theta$. The new state is made functionally identical to one of the original states. This is performed by splitting the transition probabilities to the old state between the new and the old state, and setting the transition matrix row of the new state to be the same as that of the old state. In particular, let $j'$ be the new state and $j$ be the old state, then we set the new transition probabilities $\tilde{a}$ as

$$\tilde{a}_{i,j} = \frac{1}{2}a_{i,j}, \quad \forall i \neq j'$$

$$\tilde{a}_{j',k} = \tilde{a}_{j,k}, \quad \forall k.$$  

Similarly, the initial probability for state $j$ is split with state $j'$, to form the new initial probabilities,

$$\tilde{\pi}_j = \tilde{\pi}_{j'} = \frac{1}{2}\pi_j,$$  

The old state $j$ for duplication is selected to minimize the permutation error in (22). A similar procedure occurs if $\hat{K} > K$. 


4. Experiment Setup

In the experiments, we use 10 subjects to create 10 ground-truth HMMs. The stimuli images are 512×384, with the face region roughly 300×350. We consider different numbers of samples \( N \) and sequence lengths \( T \). For each combination of \((N, T)\), we run 500 trials, where each trial randomly selects one ground-truth HMM \( \Theta \), samples \( N \) sequences of length \( T \) from which an HMM \( \hat{\Theta} \) is estimated. The ground-truth and estimated HMMs are then compared using the metrics described above: sequence KLD \( (D_{HMM}) \), matched L1-norm for ROIs \( (\ell_{ROI}) \), matched L1-norm for transitions \( (\ell_{trans}) \), and matched L1-norm for priors \( (\ell_{prior}) \).

For comparison, we also add known distortions to the parameters of a ground-truth HMM to obtain noisy HMM \( \tilde{\Theta} \), and then compute the same metrics. This allows calibration of the metrics to known distortion of the HMM parameters. In particular, we consider four types of distortion (deviation):

- **ROI Mean**: move the ROI mean by a fixed distance \( \alpha \): \( \tilde{\mu}_j = \mu_j + \alpha r \), where \( r \) is a random unit-length vector.

- **ROI Covariance**: increase or decrease the size of the covariance matrix by \( \beta \). Let \( \Sigma = VA^T \) be the eigen-decomposition. Then the covariance matrix is scaled as \( \tilde{\Sigma} = VA^{(1+\beta r)}V^T \), where random value \( r \in \{-1,1\} \) and \( \beta \) is the deviation parameter.

- **Prior Vector**: shift probability mass between states such that the L1-norm is \( \delta \), i.e., \( \psi(\pi, \tilde{\pi}) = \delta \). Specifically, \( \tilde{\pi} = \pi + \frac{2}{\delta T|r|} r \) where \( r \) is a random vector that makes \( \tilde{\pi} \) into a valid probability distribution.

- **Transition Matrix**: for each row of the transition matrix, shift probability mass between states such that the L1-norm is \( \epsilon \), i.e., \( \psi(a_j, \tilde{a}_j) = \epsilon \). Specifically, \( \tilde{a}_j = a_j + \frac{2}{\epsilon T|r|} r \), where \( r \) is a random vector that makes \( \tilde{a}_j \) into a valid probability distribution.

We compute the error metrics for HMMs using different values of the distortion parameters \( \{\alpha, \beta, \delta, \epsilon\} \), averaged over 500 trials. Then, we can interpret a particular level of error as equivalent to the corresponding level of distortion in one of the HMM parameters.

5. Experiment Results

We next present the experiment results of the simulation study.

5.1 Comparison of whole HMMs

The results for the KLD for whole HMMs is shown in Figure 1. The KLD decreases as the number of samples increases or the length of the sequences increases, and eventually converges to zero. To obtain a low KLD of 0.05 requires roughly 250 individual fixations, e.g., 52 length-5 sequences, 26 length-10 sequences, 11 length-25 sequences or 6 length-50 sequences.
Figure 1: (a) whole sequence KL divergence ($D_{HMM}$) versus number of sequences $N$ and sequence length $T$, and its equivalence to known distortion in the HMM parameters (b) mean, (c) covariance, (d) prior, (e) transition matrix.
5.2 Comparison of matched ROIs

Figure 2 shows the L1-norm between matched ROIs and its equivalent distortions in the mean and covariance parameters of the ground-truth ROI. To obtain 90% overlap (10% L1-norm) of ROIs between the two HMMs requires roughly 350 individual fixations (e.g., 66 length-5 sequences, 35 length-10 sequences, 15 length-25 sequences or 8 length-50 sequences). The total number of fixations is important since the ROIs are determined using all of the fixations from the samples. Here, 90% overlap from 350 individual fixations (e.g., 35 length-10 sequences) corresponds to roughly 4.7 pixel error in the mean or 4.5% change in the size of the ROI, as seen in Figures 2(b) and 2(c).

![Figure 2](image_url)

Figure 2: (a) L1-norm between matched ROIs ($\ell_{ROI}$), and its equivalence to known distortion in the (b) ROI mean and (c) covariance matrix.

5.3 Comparison of matched states

Figure 3 shows the L1-norm for matched states for the prior and the transition matrix, along with the equivalent distortions to the ground-truth prior and transition matrices. To obtain 90% overlap of the prior probability distribution requires 18-31 sequences (each sequence only has 1 first fixation). To obtain 90% overlap of the transition probabilities requires roughly 215 individual fixations (e.g., 43 length-5 sequences, 21 length-10 sequences,
9 length-25 sequences, or 5 length-50 sequences). Here, the total number of fixations is important since the transition matrix is computed from pairs of fixations.

![Graphs showing L1-norm of matched prior states and transition matrices](image)

Figure 3: (a) L1-norm of the matched prior states ($\ell_{\text{prior}}$) versus number of sequences $N$ and sequence length $T$, and (b) its equivalence to known distortion of the prior vector; (c) L1-norm of matched transition matrices ($\ell_{\text{trans}}$), and (d) its equivalence to known distortion of the transition matrix.

6. Summary

The results of the simulation study suggest that to obtain a low KL divergence of 0.05 between the estimated and the ground-truth HMMs requires at least 250 individual fixations. Looking at the individual components of the HMM, the results suggest that to obtain 90% overlap between the estimated and ground-truth Gaussians ROIs requires at least 350 individual fixations. To obtain 90% overlap between the transition probabilities and between the priors requires at least 215 individual fixations and 25 sequences (first fixations). Hence, any combination of sequence length and number of samples that can obtain this requirement should be able to obtain good estimates of the HMM that are close to the ground-truth.

Finally, we should note that this simulation study is testing whether estimating an HMM from samples can recover the ground-truth HMM that generated the samples. This is helpful if we want to infer the subject’s eye fixation strategy from the HMM, i.e., the subject’s underlying process that generated the observed eye fixations. However, from a
purely analysis point-of-view, it is still valid to learn HMMs from a limited set of samples, and then use the HMMs as a representation of the observed data, e.g., in a classification task as in Coutrot et al. (2018). In this case, the HMM is serving as a summarized representation of what the subject looked at in the given stimuli.

References

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