Assignment 2: HMM for Categorical Data Sequences

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1 Complete data log-likehood $l_c\left(\boldsymbol{\theta}\right)$ for the N sequences

The expression of the complete data log-likelihood will have the following form

$$l_c\left(\boldsymbol{\theta}\right) = \log p(S, Y|\boldsymbol{\theta}) = \log \prod_{n=1}^{N} \left(p\left(s_1^n|\boldsymbol{\pi}\right) \prod_{t=2}^{T_n} p\left(s_t^n|s_{t-1}^n, \mathbf{A}\right) \right) \left(\prod_{t=1}^{T_n} p\left(\mathbf{y}_t^n|s_t^n, \mathbf{B}\right) \right), \tag{1}$$

where log operator is the Naperian logarithm, S represents the hidden states of the model, Y is the observed continuous sequence, $\mathbf{A}$ stands for the state transition probabilities,B the observatoin emission probabilities and $\boldsymbol{\pi}$ is the initial state probability distribution.

The parameters of the model are

$$\boldsymbol{\theta} = \{\mathbf{A}, \mathbf{B}, \boldsymbol{\pi}\}, \tag{2}$$

where $\mathbf{A}$ is the state transition matrix, $\mathbf{B}$ is the emission matrix and $\boldsymbol{\pi}$ represents the probability of each state. Equation 1 is composed by three main terms: the $\boldsymbol{\pi}$, $\mathbf{A}$ and $\mathbf{B}$ ones which can be rewritten as

$$p\left(s_1^n|\boldsymbol{\pi}\right) = \prod_{k=1}^{K} \pi_k^{\mathbb{I}\{s_1^n=k|Y,\boldsymbol{\theta}\}}, \tag{3}$$

$$p\left(s_t^n|s_{t-1}^n, \mathbf{A}\right) = \prod_{k=1}^{K} \prod_{k'=1}^{K} a_{k,k'}^{\mathbb{I}\{s_{t-1}^n=k, s_t^n=k'|Y,\boldsymbol{\theta}\}}, \tag{4}$$

$$p\left(\mathbf{y}_t^n|s_t^n, \mathbf{B}\right) = \prod_{k=1}^{K} p\left(\mathbf{y}_t^n|\boldsymbol{b}_k\right) = \prod_{k=1}^{K} p\left(\mathbf{y}_t^n|\boldsymbol{\theta}_k\right). \tag{5}$$

In this case, $\mathbb{I}$ represents an indicator function, $k = \{1, ..., K\}$ the current latent state of the model, $a_{k,k'}$ the kth row and k'th column element of the forementioned matrix $\mathbf{A}$ and $t = \{1, ..., T_n\}$ the position of the state in sequence n. Please notice that now, $\mathbf{b}_k$ (that belonged to $\mathbf{B}$) becomes $\boldsymbol{\theta}_k$, which denotes the hyperparameters of the categorical distribution that the data follow.

Since our data follow a categorical distribution, Equation 5 can be expressed as

$$p\left(\mathbf{y}_t^n|\boldsymbol{\theta}_k\right) = \prod_{j=1}^{Dt} \mathrm{Cat}(y_{j,t}|\boldsymbol{\theta}_k). \tag{6}$$

With a further development we can get

$$p\left(\mathbf{y}_t^n|\boldsymbol{\theta}_k\right) = \prod_{j=1}^{Dt} \mathrm{Cat}(y_{j,t}|\boldsymbol{\theta}_k) = \prod_{m=1}^{I}\prod_{j=1}^{Dt} \theta_{k,m}^{\mathbb{I}\{y_{j,t}^n=m\}} = \prod_{m=1}^{I} \theta_{k,m}^{\sum_{j=1}^{Dt}\mathbb{I}\{y_{j,t}^n=m\}} = \prod_{m=1}^{I} \theta_{k,m}^{\mu_{t,m}^n}, \tag{7}$$

being $\mu_{t,m}^n$

$$\mu_{t,m}^n = \sum_{j=1}^{Dt} \mathbb{I}\{y_{j,t}^n = m\}. \tag{8}$$

The final expression of the complete data log-likelihood can be expressed in the following form

$$\begin{aligned} l_c\left(\boldsymbol{\theta}\right) = &\sum_{n=1}^{N}\sum_{k=1}^{K} \mathbb{I}\{s_1^n = k|Y,\boldsymbol{\theta}\}\log(\pi_k) + \\ &+ \sum_{n=1}^{N}\sum_{k=1}^{K}\sum_{k'=1}^{K}\sum_{t=1}^{T_n} \mathbb{I}\{s_{t-1}^n = k, s_t^n = k'|Y,\boldsymbol{\theta}\}\log(a_{k,k'}) + \\ &+ \sum_{n=1}^{N}\sum_{t=1}^{T_n} \mathbb{I}\{s_t^n = k|Y,\boldsymbol{\theta}\}\sum_{m=1}^{I} \mu_{t,m}^n \log(\theta_{k,m}). \end{aligned} \tag{9}$$

2 Expected Complete Data Logl-likelihood $Q\left(\boldsymbol{\theta}, \boldsymbol{\theta}^{t-1}\right)$

The expected complete data log-likelihood has the following form

$$Q\left(\boldsymbol{\theta}, \boldsymbol{\theta}^{t-1}\right) = E\left\{l_c(\boldsymbol{\theta})|\mathcal{D}, \boldsymbol{\theta}^{t-1}\right\} \tag{10}$$

As in the previous section, and considering the nature of l_c and its three main components, this expectation calculation can be divided in three.

$$\mathbb{E}\left(\sum_{n=1}^{N} \mathbb{I}\left(s_1^n = k|Y,\boldsymbol{\theta}\right)\right) = \sum_{n=1}^{N} \gamma_{n,1}(k), \tag{11}$$

$$\mathbb{E}\left(\sum_{n=1}^{N}\sum_{t=2}^{T_n} \mathbb{I}\left(s_{t-1}^n = k, s_t^n = k'|Y,\boldsymbol{\theta}\right)\right) = \sum_{n=1}^{N}\sum_{t=2}^{T_n} \xi_{n,t}(k,k'), \tag{12}$$

$$\mathbb{E}\left(\sum_{n=1}^{N}\sum_{t=1}^{T_n} \mathbb{I}\left(s_t^n = k|Y,\boldsymbol{\theta}\right)\right) = \sum_{n=1}^{N}\sum_{t=1}^{T_n} \gamma_{n,t}(k). \tag{13}$$

Where

$$\sum_{k=1}^{K} \gamma_{n,t}(k) = 1. \tag{14}$$

Being $\xi_{n,t}(k,k')$

$$\xi_{n,t}(k,k') = \alpha_{t-1}^{n}(k) a_{k,k'} \prod_{m=1}^{I} \theta_{k,m}^{\mu_{t,m}^{n}} \beta_{t}^{n}(k'), \tag{15}$$

and $\gamma_{n,t}(k)$

$$\gamma_{n,t}(k) \propto \beta_{t}^{n}(k) \alpha_{t}^{n}(k) \tag{16}$$

The terms α and β are computed by means of the **forward-backward algorithm** as follows

$$\begin{align}
\alpha_{1}^{n}(k) &= \pi_k \prod_{m=1}^{I} \theta_{k,m}^{\mu_{1,m}^{n}}, \tag{17}\\
\alpha_{t}^{n}(k) &= \left(\sum_{k'=1}^{K} \alpha_{t-1}^{n}(k') a_{k',k} \right) \prod_{m=1}^{I} \theta_{k,m}^{\mu_{t,m}^{n}}, \tag{18}\\
\beta_{T_n}^{n}(k) &= 1, \tag{19}\\
\beta_{t}^{n}(k) &= \sum_{k'=1}^{K} a_{k,k'} \prod_{m=1}^{I} \theta_{k',m}^{\mu_{t+1,m}^{n}} \beta_{t+1}^{n}(k'). \tag{20}
\end{align}$$

So the complete expression for $Q\left(\boldsymbol{\theta}, \boldsymbol{\theta}^{t-1}\right)$ is now

$$\begin{aligned}
Q\left(\boldsymbol{\theta}, \boldsymbol{\theta}^{t-1}\right) = & \sum_{k=1}^{K} \sum_{n=1}^{N} \gamma_{n,1}(k) \log(\pi_k) + \\
& + \sum_{k=1}^{K} \sum_{k'=1}^{K} \sum_{n=1}^{N} \sum_{t=2}^{T_n} \xi_{n,t}(k,k') \log(a_{k,k'}) + \\
& + \sum_{k=1}^{K} \sum_{m=1}^{I} \sum_{n=1}^{N} \sum_{t=1}^{T_n} \gamma_{n,t}(k) \mu_{t,m}^{n} \log(\theta_{k,m}).
\end{aligned} \tag{21}$$

3 ML Inference

There are three parameters for the model, which are $\mathbf{A}$, $\boldsymbol{\theta}$ and $\boldsymbol{\pi}$, and they are computed by means of Lagrange multipliers.

3.1 ML estimation of π_k

In order to compute π_k, we first need to take into account the following restrictions

$$\begin{align}
0 \leq \pi_k \leq 1 \tag{22}\\
\sum_{k=1}^{K} \pi_k = 1. \tag{23}
\end{align}$$

Now, let us define the lagrangian as

$$L\left(Q(\pi_k), \lambda\right) = Q(\pi_k) + \lambda \left(\sum_{k=1}^{K} \pi_k - 1 \right), \tag{24}$$

which will be optimized in this way

$$\min_{\lambda} \max_{\pi_k} \{ L\left(Q(\pi_k), \lambda\right) \}. \tag{25}$$

By first taking the derivative with respect to π_k and equating it to 0

$$\begin{aligned} \frac{\partial L}{\partial \pi_k} &= \sum_{n=1}^{N} \frac{\gamma_{n,1}(k)}{\pi_k} - \lambda = 0, \\ \pi_k &= \frac{1}{\lambda} \sum_{n=1}^{N} \gamma_{n,1}(k). \end{aligned} \tag{26}$$

And later with respect to λ

$$\begin{aligned} \frac{\partial L}{\partial \lambda} &= \sum_{k=1}^{K} \pi_k - 1 = 0, \\ \sum_{k=1}^{K} \pi_k &= 1. \end{aligned} \tag{27}$$

Taking into account the previous equation, if in both sides of Equation 26 summatories all over K are taken, then the value of λ can be obtained

$$\begin{aligned} \sum_{k=1}^{K} \pi_k &= \sum_{k=1}^{K} \frac{1}{\lambda} \sum_{n=1}^{N} \gamma_{n,1}(k) \\ 1 &= \frac{1}{\lambda} \sum_{n=1}^{N} \sum_{k=1}^{K} \gamma_{n,1}(k). \end{aligned} \tag{28}$$

Now, considering the previously imposed restrictions and recalling that

$$\sum_{k=1}^{K} \gamma_{n,t}(k) = 1, \tag{29}$$

the value of λ is

$$\begin{aligned} 1 &= \frac{1}{\lambda} \sum_{n=1}^{N} 1. \\ \lambda &= N. \end{aligned} \tag{30}$$

And with that value of λ the estimated value of π_k is

$$\widehat{\pi}_k = \frac{1}{N} \sum_{n=1}^{N} \gamma_{n,1}(k). \tag{31}$$

3.2 ML estimation of $\theta_{k,m}$

Now, the parameter to be estimated is $\theta_{k,m}$ and the constraint is now

$$\sum_{m=1}^{I} \theta_{k,m} = 1. \tag{32}$$

Being the whole expression

$$L\left(Q(\theta_{k,m}), \lambda\right) = Q(\theta_{k,m}) + \lambda \left(\sum_{m=1}^{I} \theta_{k,m} - 1 \right), \tag{33}$$

which will be optimized in this way

$$\min_{\lambda} \max_{\theta_{k,m}} \{ L\left(Q(\theta_{k,m}), \lambda\right) \}. \tag{34}$$

By first taking the derivative with respect to $\theta_{k,m}$ and equating it to 0

$$\begin{aligned} \frac{\partial L}{\partial \theta_{k,m}} &= \sum_{n=1}^{N} \sum_{t=1}^{T_n} \frac{\gamma_{n,t}(k) \mu_{t,m}^{n}}{\theta_{k,m}} - \lambda = 0, \\ \theta_{k,m} &= \frac{1}{\lambda} \sum_{n=1}^{N} \sum_{t=1}^{T_n} \gamma_{n,t}(k) \mu_{t,m}^{n}. \end{aligned} \tag{35}$$

And later with respect to λ

$$\begin{aligned} \frac{\partial L}{\partial \lambda} &= \sum_{m=1}^{I} \theta_{k,m} - 1 = 0, \\ \sum_{m=1}^{I} \theta_{k,m} &= 1. \end{aligned} \tag{36}$$

Taking into account the previous equation, if in both sides of Equations 35 summatories all over I are taken, then the value of λ can be obtained

$$\begin{aligned} \sum_{m=1}^{I} \theta_{k,m} &= \sum_{m=1}^{I} \frac{1}{\lambda} \sum_{n=1}^{N} \sum_{t=1}^{T_n} \gamma_{n,t}(k) \mu_{t,m}^{n} \\ 1 &= \frac{1}{\lambda} \sum_{n=1}^{N} \sum_{t=1}^{T_n} \sum_{m=1}^{I} \gamma_{n,t}(k) \mu_{t,m}^{n}, \\ \lambda &= \sum_{n=1}^{N} \sum_{t=1}^{T_n} \sum_{m=1}^{I} \gamma_{n,t}(k) \mu_{t,m}^{n}. \end{aligned} \tag{37}$$

And with that value of λ the estimated value of $\theta_{k,m}$ is

$$\widehat{\theta}_{k,m} = \frac{\sum\limits_{n=1}^{N} \sum\limits_{t=1}^{T_n} \gamma_{n,t}(k) \mu_{t,m}^{n}}{\sum\limits_{n=1}^{N} \sum\limits_{t=1}^{T_n} \sum\limits_{m=1}^{I} \gamma_{n,t}(k) \mu_{t,m}^{n}}. \tag{38}$$

3.3 ML estimation of $a_{k,k'}$

At last, the parameter to be estimated is $a_{k,k'}$ and the constraint is now

$$\sum_{k'=1}^{K} a_{k,k'} = 1. \tag{39}$$

Being the whole expression

$$L\left(Q(a_{k,k'}), \lambda\right) = Q(a_{k,k'}) + \lambda \left(\sum_{k'=1}^{K} a_{k,k'} - 1 \right), \tag{40}$$

which will be optimized in this way

$$\min_{\lambda} \max_{a_{k,k'}} \{ L\left(Q(a_{k,k'}), \lambda\right) \}. \tag{41}$$

By first taking the derivative with respect to $a_{k,k'}$ and equating it to 0

$$\begin{aligned} \frac{\partial L}{\partial a_{k,k'}} &= \sum_{n=1}^{N} \sum_{t=2}^{T_n} \frac{\xi_{n,t}(kk')}{a_{k,k'}} - \lambda = 0, \\ a_{k,k'} &= \frac{1}{\lambda} \sum_{n=1}^{N} \sum_{t=2}^{T_n} \xi_{n,t}(kk'). \end{aligned} \tag{42}$$

And later with respect to λ

$$\begin{aligned} \frac{\partial L}{\partial \lambda} &= \sum_{m=1}^{I} a_{k,k'} - 1 = 0, \\ \sum_{k'=1}^{K} a_{k,k'} &= 1. \end{aligned} \tag{43}$$

Taking into account the previous equation, if in both sides of (42) summatories all over I are taken, then the value of λ can be obtained

$$\begin{aligned} \sum_{k'=1}^{K} a_{k,k'} &= \sum_{k'=1}^{K} \frac{1}{\lambda} \sum_{n=1}^{N} \sum_{t=1}^{T_n} \xi_{n,t}(k,k') \\ 1 &= \frac{1}{\lambda} \sum_{n=1}^{N} \sum_{t=1}^{T_n} \sum_{k'=1}^{K} \xi_{n,t}(k,k'), \\ \lambda &= \sum_{n=1}^{N} \sum_{t=1}^{T_n} \sum_{k'=1}^{K} \xi_{n,t}(k,k'). \end{aligned} \tag{44}$$

And with that value of λ the estimated value of $a_{k,k'}$ is

$$\widehat{a}_{k,k'} = \frac{\sum_{n=1}^{N} \sum_{t=1}^{T_n} \xi_{n,t}(k,k')}{\sum_{n=1}^{N} \sum_{t=1}^{T_n} \sum_{k'=1}^{K} \xi_{n,t}(k,k')}. \tag{45}$$

4 State Decoder

Each document in each sequence has been generated by some state of the HMM. In the following section we present the two types of decoding algorithms that have been used to find such states: the state-by-state MAP decoding based on the Forward-Backwards algorithm and the ML iterative Viterbi algorithm.

4.1 MAP decoding based on Forward-Backwards

In order to determine the state of each document for the different sequences we obtain the most probable state for each document at each sequence from the parameter $\gamma_{n,t}(k)$ which is computed in the E-step of the Baum-Welch EM using Equation 16.

4.2 ML Viterbi decoding

As a comparison for the MAP decoding comment above, we have also implemented a Viterbi decoder. The Viterbi decoder is a dynamic programming algorithm for finding the most likely sequence of hidden states result of a sequence of observed events. Since we are dealing with hidden and observed states with HMM, the algorithm suits perfectly to our problem. The Viterbi decoding algorithm looks as follows

$$\underset{S}{\operatorname{argmax}} p(S,Y) = \underset{i}{\operatorname{argmax}} \left\{ \underset{s_{1:T-1}}{\operatorname{argmax}} p\left(s_T = i, s_{1:T-1}, Y\right) \right\}. \tag{46}$$

In particular, we will use an iterative implementation of the Viterbi Algorithm. For such implementation we define two iterative steps described below.

- **Forward step**: Computed with the following equations

$$\delta_1(k) = \pi_k \prod_{m=1}^{I} \theta_{k,m}^{\mu_{1,m}^n} \quad 1 \le k \le K \tag{47}$$

$$\delta_t(k) = \prod_{m=1}^{I} \theta_{k,m}^{\mu_{t,m}^n} \max_{k'} a_{k',k} \delta_{t-1}(k') \quad 1 \le k \le K, 1 \le t \le T \tag{48}$$

$$\varphi_t(k) = \underset{k'}{\operatorname{argmax}}\, a_{k',k} \delta_{t-1}(k') \quad 1 \le k \le K, 1 \le t \le T \tag{49}$$

$$\tag{50}$$

- **Backwards step**: The state estimation is computed using the following Equations

$$\hat{\mathbf{s}}_T = \arg \max_{\boldsymbol{k}} \delta_T(k) \tag{51}$$

$$\hat{s}_t = \varphi_{t+1}\left(\hat{s}_{t+1}\right) 1 \le t \le T. \tag{52}$$

	2	3	4	5
A	$\begin{bmatrix} 0.32 & 0.68 \\ 0.37 & 0.63 \end{bmatrix}$	$\begin{bmatrix} 0.64 & 0.18 & 0.18 \\ 0.44 & 0.20 & 0.36 \\ 0.38 & 0.44 & 0.18 \end{bmatrix}$	$\begin{bmatrix} 0.2 & 0.27 & 0.43 & 0.1 \\ 0.21 & 0.30 & 0.13 & 0.36 \\ 0.1 & 0.35 & 0.34 & 0.21 \end{bmatrix}$	$\begin{bmatrix} 0.02 & 0.22 & 0.36 & 0.34 & 0.06 \\ 0.07 & 0.16 & 0.21 & 0.21 & 0.35 \\ 0.12 & 0.11 & 0.44 & 0.15 & 0.18 \\ 0.32 & 0.22 & 0.35 & 0.1 & 0.01 \\ 0.26 & 0.14 & 0.30 & 0.20 & 0.10 \end{bmatrix}$
π	$\begin{bmatrix} 0.28 & 0.72 \end{bmatrix}$	$\begin{bmatrix} 0.14 & 0.30 & 0.56 \end{bmatrix}$	$\begin{bmatrix} 0.34 & 0.38 & 0.28 & 1.27e^{-80} \end{bmatrix}$	$\begin{bmatrix} 0.48 & 0.38 & 6.46e^{-80} & 1.12e^{-103} & 0.13 \end{bmatrix}$

5 Experiments

One **important** aspect about the implementation of the algorithm is that instead of working with the actual $\xi_{n,t}(k,k')$ we work with a similar implementation used in [1], which consider working with the expected sufficient statistics for the transition matrix, for a given observation sequence. This may be rewritten as follows

$$\xi_{\Sigma}(k,k') = \sum_{t=2}^{T} p(S(t)=k, S(t+1)=k'|y(1:T)), \tag{53}$$

where the subscript Σ indicates the sum over t. Notice that, for a given sequence, this matrix is no longer a tensor but a matrix of dimension $K \times K$.

5.1 Simulations

In Figure 1 we show first all the log-likelihoods together, where one can infer that the best case happens for K = 5 since it gives the curve with the biggest values.

Next, Figure 2 displays like Figure 1 all log-likelihood curves but in this case separated.

This last set of figures, which include from Figure 3 until Figure 6, show the estimated states for sequences for K ∈ [2,5].

6 Final Thoughts

By looking at the plots, we can see a proper behaviour of of the curves (which begin growing up and later they stabilize around some fixed value) and the algorithms. Both experiments seem to have a similar performance, they show that they reach almost always the same states for all the sequences. And at last, a bigger number of K increases the complexity of the model, which includes the number of states among other things, but gives a better performance with a bigger log-likelihood curve.

References

[1] K. P. Murphy, *Machine learning: A probabilistic perspective. adaptive computation and machine learning*, 2012.

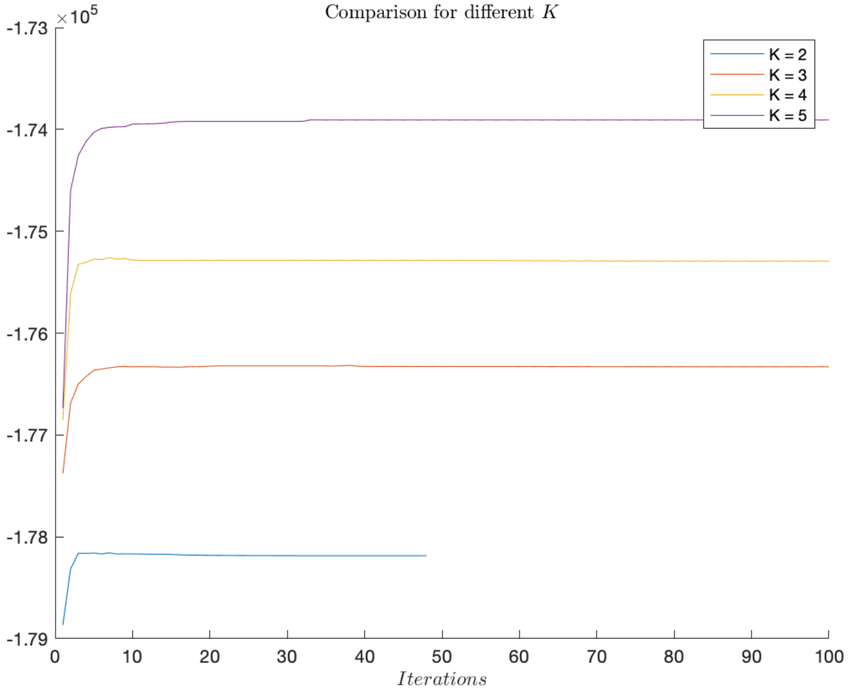


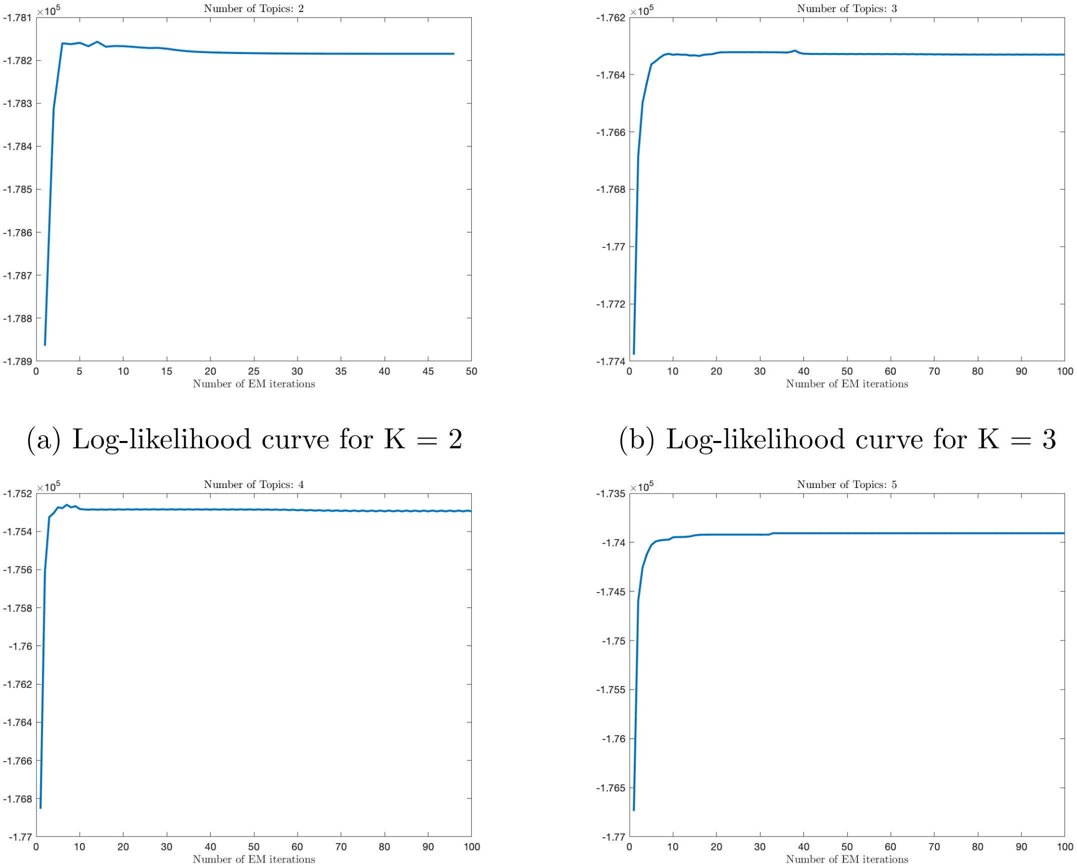
Figure 1. Comparison of the log-likelihoods for K ∈ [2,5]

[2] C. Fraley and A. E. Raftery, "Bayesian regularization for normal mixture estimation and model-based clustering," *Journal of classification*, vol. 24, no. 2, pp. 155–181, 2007.

[3] C. M. Bishop, *Pattern Recognition and Machine Learning*. Springer, 2006. [Online]. Available: http://research.microsoft.com/en-us/um/people/cmbishop/prml/.

[4] A. Artés-Rodríguez, *Notes for advanced signal processing*, 2018.

[5] R. Eisele, *The log-sum-exp trick in machine learning*. [Online]. Available: https://www.xarg.org/2016/06/the-log-sum-exp-trick-in-machine-learning/.



(a) Log-likelihood curve for K = 2

(b) Log-likelihood curve for K = 3

(c) Log-likelihood curve for K = 4

(d) Log-likelihood curve for K = 5

Figure 2. Separated log-likelihood curves for K $\in$ [2,5]

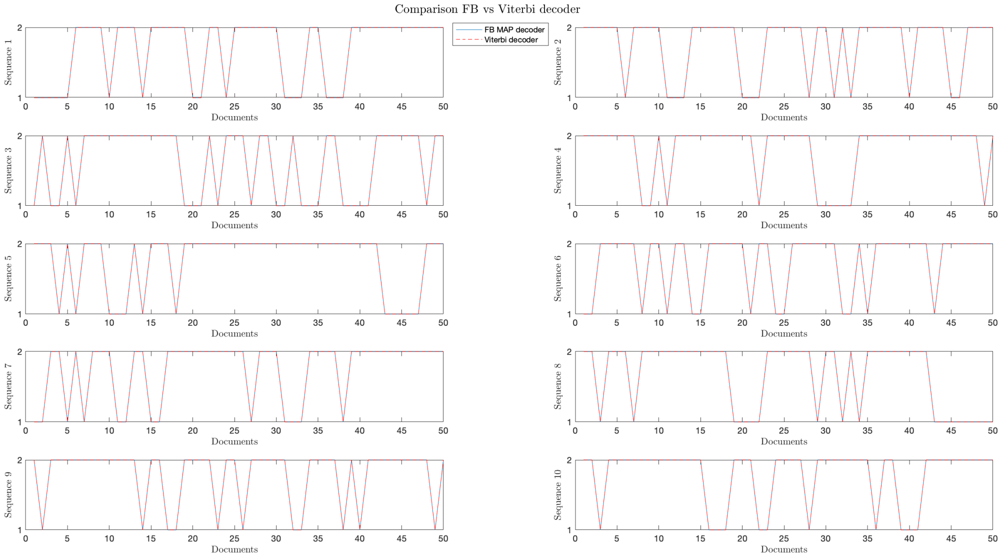


Figure 3. Forward Backward (MAP) and Viterbi (ML) estimations for K = 2

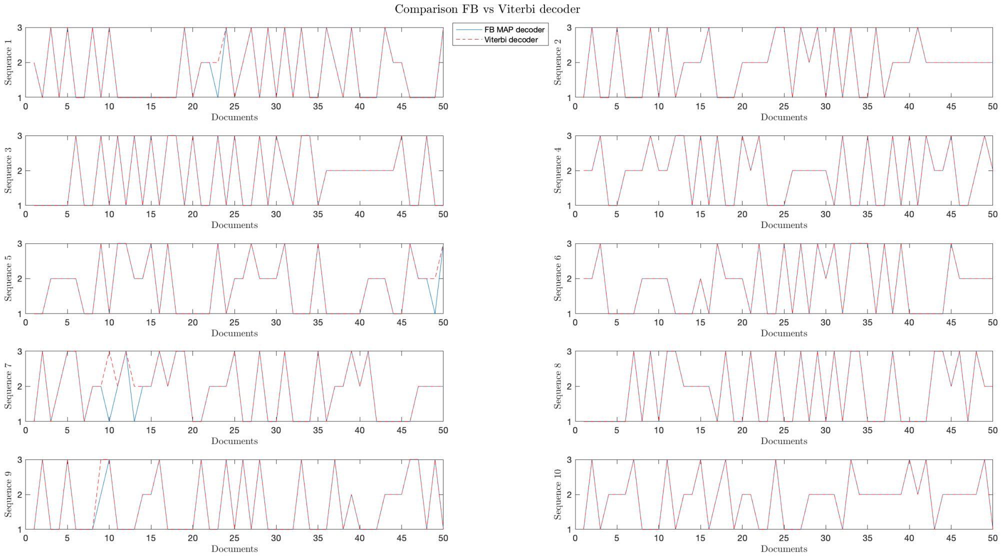


Figure 4. Forward Backward (MAP) and Viterbi (ML) estimations for K = 3

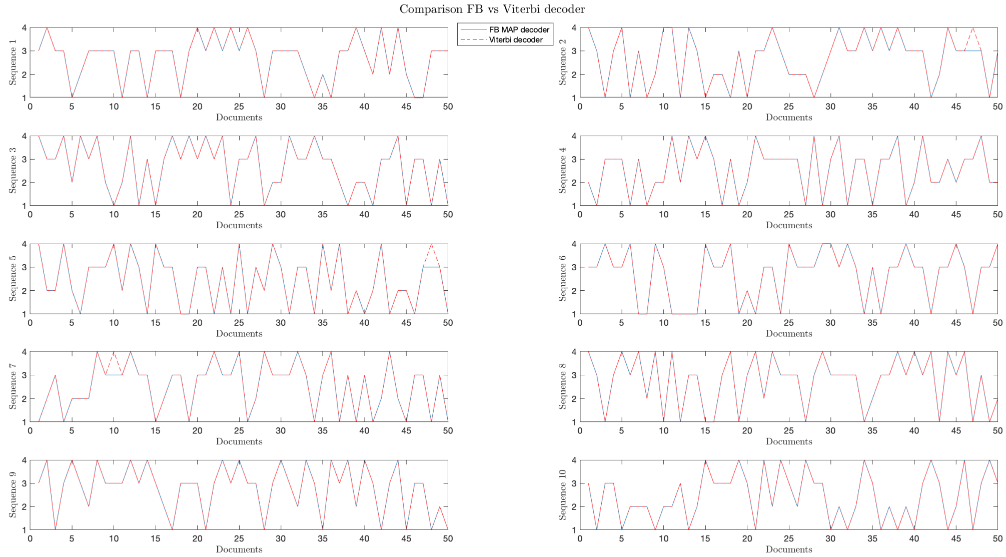


Figure 5. Forward Backward (MAP) and Viterbi (ML) estimations for K = 4

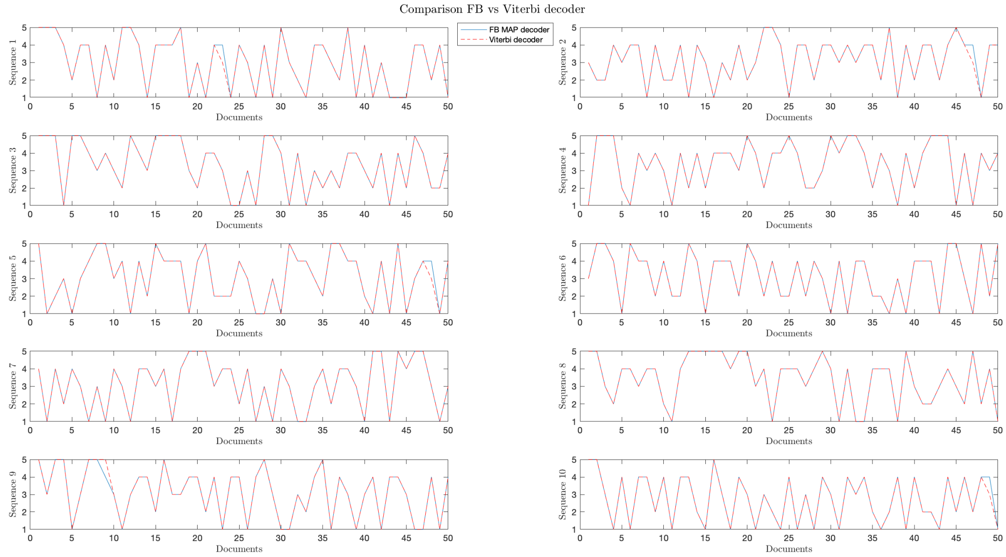


Figure 6. Forward Backward (MAP) and Viterbi (ML) estimations for K = 5