Assignment 2: HMM for Categorical Data Sequences

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1 Expression for the complete data log-likehood for the N sequences

According to this expression for the complete data log-likelihood

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

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 probabilites and $\boldsymbol{\pi}$ is the initial state probability distribution.

The parameters of the model are

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

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 $\mathbf{A}$, $t = \{1, ..., T_n\}$ 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 $\mu_{t,m}^n$

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

So the complete data log-likelihood is written in this way

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

2 Expression for the expected complete data log likelihood

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

$$\alpha_1^n(k) = \pi_k \prod_{m=1}^{I} \theta_{k,m}^{\mu_{1,m}^n}, \tag{17}$$

$$\alpha_t^n(k) = \left(\sum_{k'=1}^{K} \alpha_{t-1}^n(k') a_{k',k} \right) \prod_{m=1}^{I} \theta_{k,m}^{\mu_{t,m}^n}, \tag{18}$$

$$\beta_{T_n}^n(k) = 1, \tag{19}$$

$$\beta_t^n(k) = \sum_{k'=1}^{K} a_{k,k'} \prod_{m=1}^{I} \theta_{k',m}^{\mu_{t+1,m}^n} \beta_{t+1}^n(k'). \tag{20}$$

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 Maximum Likelihood estimation of the parameters of the model

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

$$0 \leq \pi_k \leq 1 \tag{22}$$

$$\sum_{k=1}^{K} \pi_k = 1. \tag{23}$$

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

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

And later with respect to λ

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

Taking into account the previous equation, if in both sides of (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

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

And later with respect to λ

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

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

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

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

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

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

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

And later with respect to λ

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

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

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

4 Experiments

The experiments that have been done include 100 iterations, with a tolerance value of 10^{-3} and with 30 initializations.

4.1 MAP decoding

The state-by-state MAP decoding has been developed with the forward-backward algorithm, whose parameters $\alpha_t^n(k)$ and $\beta_t^n(k)$ have been computed as stated in (17) and following.

4.2 ML decoding

For the maximum likelihood sequence decoding a Viterbi algorithm has been implemented. The required parameters $\delta_t(i)$, $\varphi_t(i)$, and the detected states $\hat{s}_t$ are defined as follows.

$$\delta_1(k) = \pi_k \prod_{m=1}^{I} \theta_{k,m}^{\mu_{1,m}^n} \tag{46}$$

$$\delta_t(k) = \prod_{m=1}^{I} \theta_{k,m}^{\mu_{t,m}^n} \max_{k'} a_{k',k} \delta_{t-1}(k') \tag{47}$$

$$\varphi_t(k) = \underset{k'}{\operatorname{argmax}}\, a_{k',k} \delta_{t-1}(k') \tag{48}$$

$$\hat{\mathbf{s}}_T = \arg\max_{\boldsymbol{k}} \delta_T(k) \tag{49}$$

$$\hat{s}_t = \varphi_{t+1}\left(\hat{s}_{t+1}\right) \tag{50}$$

4.3 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.

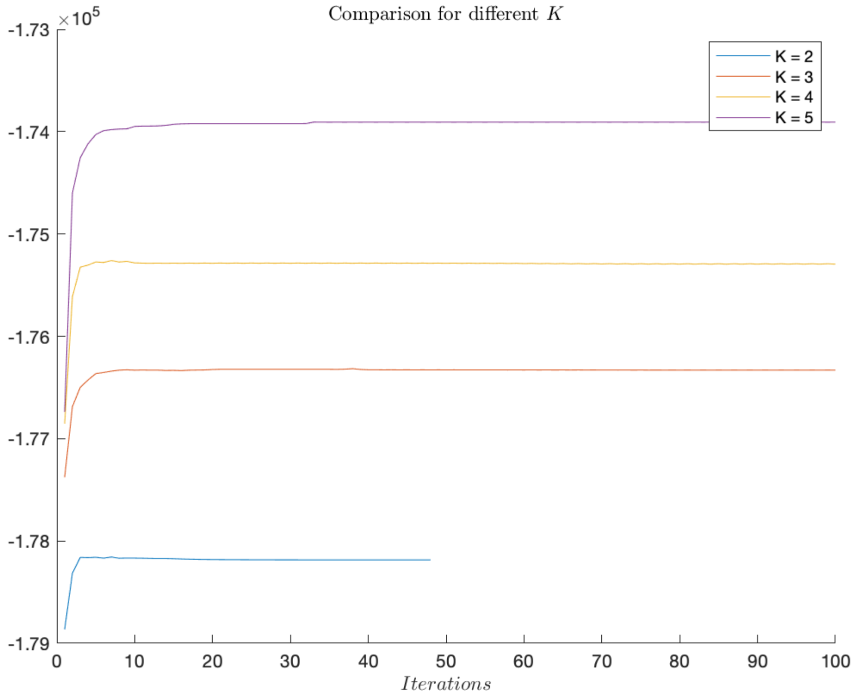
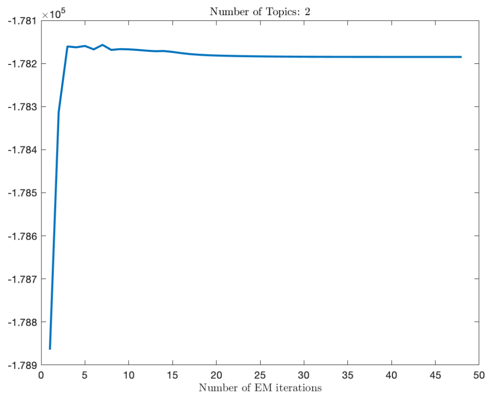
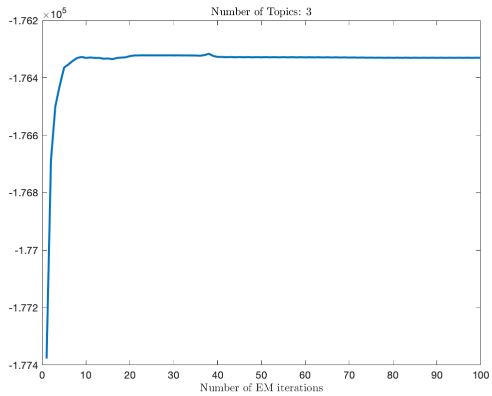


Figure 1: Comparison of the log-likelihoods for K $\in$ [2,5]

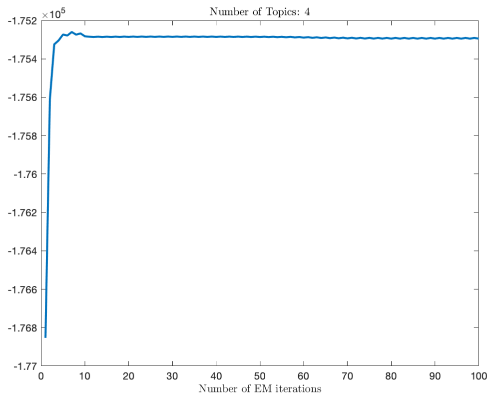
Next, Figure 2 displays like Figure 1 all log-likelihood curves but in this case separated.



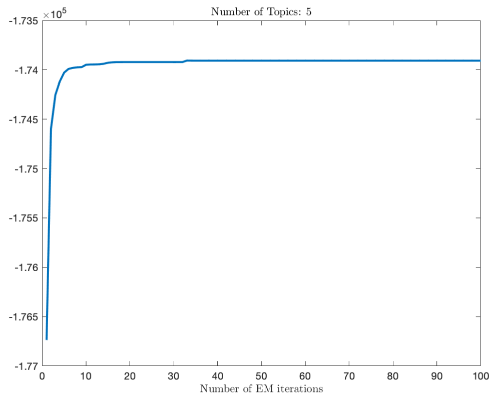
(a) Log-likelihood curve for K = 2



(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]

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

5 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.

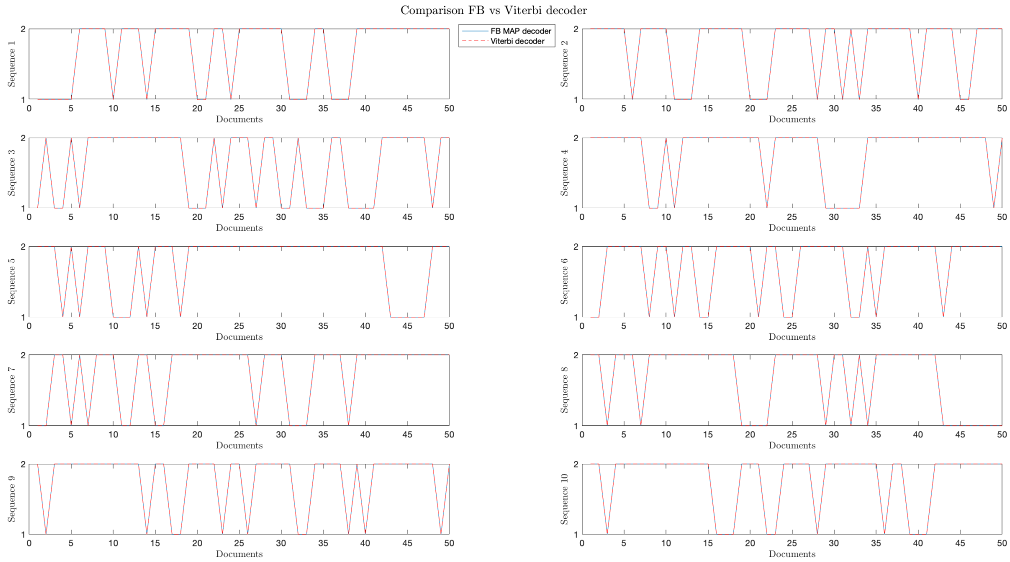


Figure 3: Forward Backward (MAP) and Viterbi (ML) estimations for K = 2

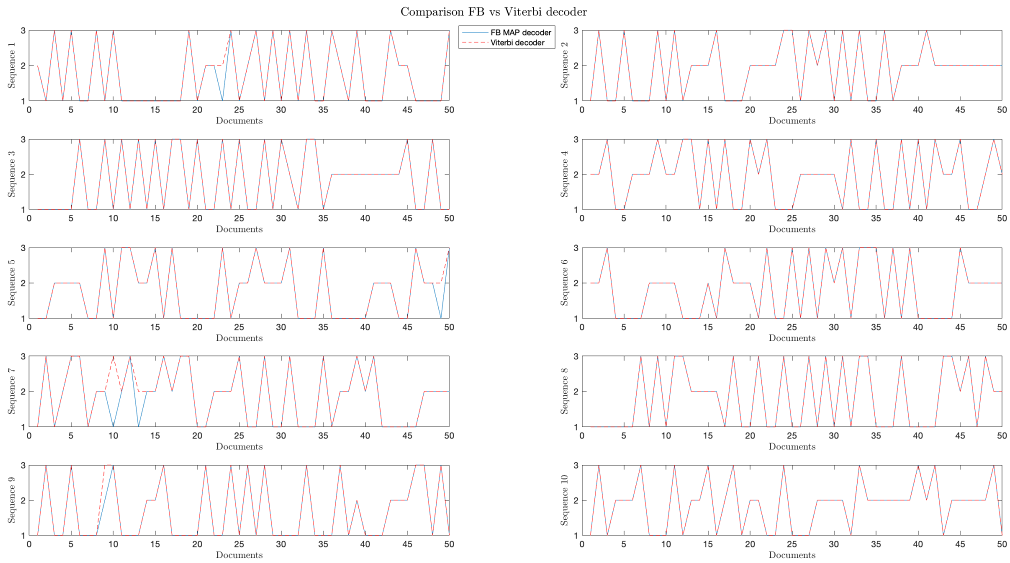


Figure 4: Forward Backward (MAP) and Viterbi (ML) estimations for K = 3

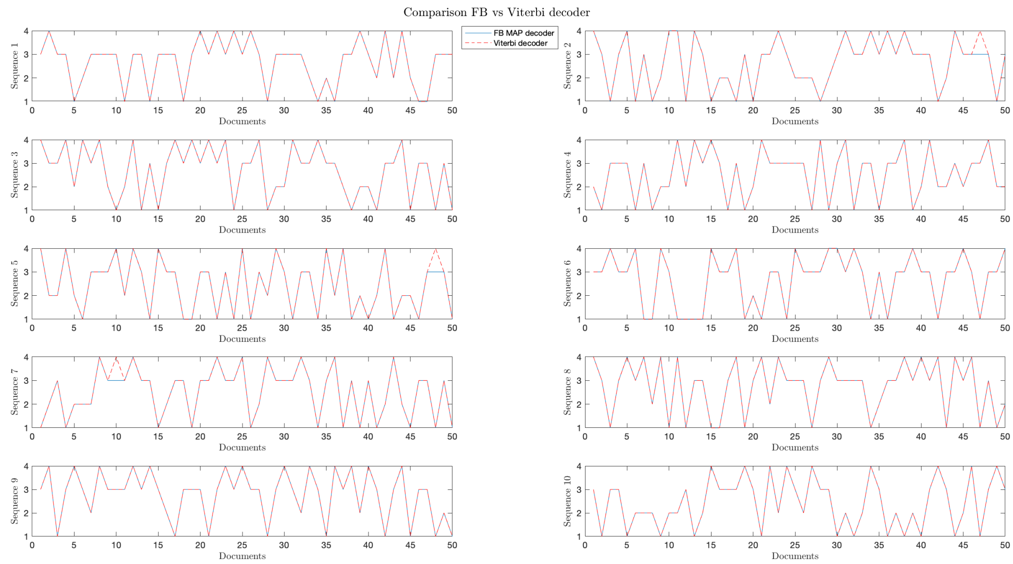


Figure 5: Forward Backward (MAP) and Viterbi (ML) estimations for K = 4

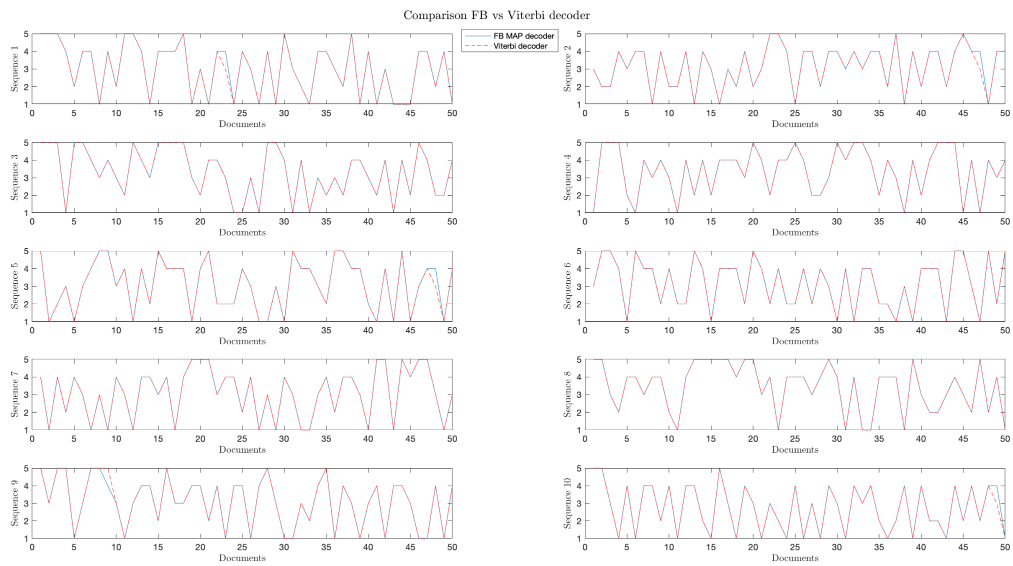


Figure 6: Forward Backward (MAP) and Viterbi (ML) estimations for K = 5