EE613 - Machine Learning for Engineers

HIDDEN MARKOV MODELS

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Learning from demonstration

EE613 labs: Tobias Löw



EE613 schedule

Thu. 21.09.2023	(C) 1. ML introduction
Thu. 28.09.2023	(C) 2. Bayesian 1 (C) 3. Bayesian 2
Thu. 12.10.2023	(C) 4. Hidden Markov Models
Thu. 19.10.2023	(C) 5. Dimensionality reduction
Thu. 26.10.2023	(C) 6. Decision trees
Thu. 02.11.2023	(C) 7. Linear regression
Thu. 09.11.2023	(C) 8. Nonlinear regression
Thu. 16.11.2023	(C) 9. Kernel Methods - SVM
Thu. 23.11.2023	(C) 10. Tensor factorization
Thu. 30.11.2023	(C) 11. Deep learning 1
Thu. 07.12.2023	(C) 12. Deep learning 2
Thu. 14.12.2023	(C) 13. Deep learning 3
Thu. 21.12.2023	(C) 14. Deep learning 4

Recap from 28/09 lecture (Jean-Marc)

Overview

- Graphical models fundamentals
 - Bayesian networks, representations
 - conditional independence
 - undirected graphical models

Learning

- ML, MAP, Bayesian
- the EM algorithm, latent variable models
 - Gaussian Mixture Model (GMM)
 - Hidden Markov Model (HMM)
- Later : PCA, Probabilistic PCA





Recap: Local optima issue when using EM for GMM







Recap: Local optima issue when using EM for GMM



Recap: Local optima issue when using EM for GMM



Hidden Markov Model (HMM)



Lattice representation of a sequence of observations (with the possible associated hidden states) Dictionary



Dictionary of possible observations



Options for the underlying hidden states $S_{1:6}$



GMM vs HMM



- \rightarrow You can think of an HMM either as:
 - a Markov chain with stochastic measurements
 - a GMM with transition between the Gaussians

Outline of today's lecture

- Markov models
- Hidden Markov model (HMM)
- Forward-backward algorithm
- Viterbi decoding (dynamic programming)
- Hidden semi-Markov model (HSMM)
- HMM with dynamic features (Trajectory-HMM)

Markov models



With a **first order Markov model**, the joint distribution of a sequence of states is assumed to be of the form

$$\mathcal{P}(s_1, s_2, \dots, s_T) = \mathcal{P}(s_1) \prod_{t=2}^T \mathcal{P}(s_t | s_{t-1})$$

and we thus have

$$\mathcal{P}(s_t|s_1, s_2, \dots, s_{t-1}) = \mathcal{P}(s_t|s_{t-1})$$

In most applications, the conditional distributions $\mathcal{P}(s_t|s_{t-1})$ will be assumed to be **stationary** (homogeneous Markov chain).

Markov models - Parameters

The **initial state distribution** is defined by

$$\Pi_i = \mathcal{P}(s_1 = i) \quad \text{with} \quad \sum_{i=1}^K \Pi_i = 1$$

A transition matrix A is defined, with elements

$$a_{i,j} = \mathcal{P}(s_{t+1} = j \mid s_t = i)$$

defining the probability of getting from state i to state j in one step.

Constraint: each row of the matrix sums to one, $\sum_{j=1}^{K} a_{i,j} = 1$.

K possible states





	1	2	3			
1	$a_{1,1}$	$a_{1,2}$	$a_{1,3}$			
2	$a_{2,1}$	$a_{2,2}$	$a_{2,3}$			
3	$a_{3,1}$	$a_{3,2}$	$a_{3,3}$			

Example: language modeling

We define the state space to be all the words in some language.

The marginal probabilities $\mathcal{P}(s_t = k)$ are called **unigram** statistics.

For a first-order Markov model, $\mathcal{P}(s_t = k \mid s_{t-1} = j)$ is called a **bigram** model.

For a second-order Markov model, $\mathcal{P}(s_t = k \mid s_{t-1} = j, s_{t-2} = i)$ is called a **trigram** model, etc.

In the general case, these are called n-gram models.

Example: language modeling

Sentence completion

The model can predict the next word given the previous words in a sentence. This can be used to reduce the amount of typing required (e.g., mobile devices).

Data compression

The model can be used to define an encoding scheme, by assigning codewords to more probable strings. The more accurate the predictive model, the fewer the number of bits is required to store the data.

Text classification

The model can be used as a class-conditional density and/or generative classifier.

Automatic writing

The model can be used to sample from $\mathcal{P}(s_1, s_2, \ldots, s_t)$ to generate artificial text.

Example: language modeling

SAYS IT'S NOT IN THE CARDS LEGENDARY RECONNAISSANCE BY ROLLIE DEMOCRACIES UNSUSTAINABLE COULD STRIKE REDLINING VISITS TO PROFIT BOOKING WAIT HERE AT MADISON SQUARE GARDEN COUNTY COURTHOUSE WHERE HE HAD BEEN DONE IN THREE ALREADY IN ANY WAY IN WHICH A TEACHER ...

Example of text generated from a 4-gram model, trained on a corpus of 400 million words.

The first 4 words are specified by hand, the model generates the 5th word, and then the results are fed back into the model.

Source: http://www.fit.vutbr.cz/~imikolov/rnnlm/gen-4gram.txt

MLE of transition matrix in Markov models

A Markov model is described by $\Theta^{MM} = \{\{a_{i,j}\}_{j=1}^K, \Pi_i\}_{i=1}^K$, where the transition probabilities $a_{i,j}$ are stored in a matrix A.

The maximum likelihood estimate (MLE) of the parameters can be computed with the normalized counts

$$\hat{\Pi}_{i} = \frac{N_{i}}{\sum_{k=1}^{K} N_{k}}, \qquad \hat{a}_{i,j} = \frac{N_{i,j}}{\sum_{k=1}^{K} N_{i,k}}$$

These results can be extended to higher order Markov models, but since an n-gram models has $O(K^n)$ parameters, special care needs to be taken with overfitting.

For example, with a bi-gram model and 50,000 words in the dictionary, there are 2.5 billion parameters to estimate, and it is unlikely that all possible transitions will be observed in the training data.

Hidden Markov model (HMM)

> Python notebook: demo_HMM.ipynb

Matlab code: demo_HMM01.m

Emission/output distributions in HMM



GMM with latent variable \boldsymbol{z}_t depending on the conditional distribution $\mathcal{P}(\boldsymbol{z}_t | \boldsymbol{z}_{t-1})$

Transition matrix structures in HMM



HMM - Examples of application

HMM is used in many fields as a tool for **time series or sequences analysis**, and in fields where the goal is to recover a data sequence that is not immediately observable:

Speech recognition Speech synthesis Part-of-speech tagging Natural language modeling Machine translation Gene prediction Molecule kinetic analysis DNA motif discovery Alignment of bio-sequences (e.g., proteins) Metamorphic virus detection Document separation in scanning solutions

Cryptoanalysis Activity recognition Protein folding Human motion science Online handwriting recognition Robotics



HMM parameters

$$egin{aligned} &oldsymbol{\Theta}^{\scriptscriptstyle ext{GMM}} = \{\pi_i, oldsymbol{\mu}_i, oldsymbol{\Sigma}_i\}_{i=1}^K \ &oldsymbol{\Theta}^{\scriptscriptstyle ext{HMM}} = \{\{a_{i,j}\}_{j=1}^K, \Pi_i, oldsymbol{\mu}_i, oldsymbol{\Sigma}_i\}_{i=1}^K \end{aligned}$$

From now on, we will consider a single Gaussian as state output

$$\pi_i = 1$$



Inference problems associated with HMMs

Probability of an observed sequence $\mathcal{P}(\boldsymbol{\xi}_{1:T}) = \mathcal{P}(\boldsymbol{\xi}_1, \boldsymbol{\xi}_2, \dots, \boldsymbol{\xi}_T)$

Probability of the latent variables

Filtering $\mathcal{P}(s_t | \boldsymbol{\xi}_{1:t}) = \mathcal{P}(s_t | \boldsymbol{\xi}_1, \boldsymbol{\xi}_2, \dots, \boldsymbol{\xi}_t)$

Prediction $\mathcal{P}(s_{t+1} | \boldsymbol{\xi}_{1:t}) = \mathcal{P}(s_{t+1} | \boldsymbol{\xi}_1, \boldsymbol{\xi}_2, \dots, \boldsymbol{\xi}_t)$

Smoothing \rightarrow Forward-backward algorithm $\mathcal{P}(s_t | \boldsymbol{\xi}_{1:T}) = \mathcal{P}(s_t | \boldsymbol{\xi}_1, \boldsymbol{\xi}_2, \dots, \boldsymbol{\xi}_T)$

MAP estimation \rightarrow Viterbi decoding $\mathcal{P}(s_{1:T} | \boldsymbol{\xi}_{1:T}) = \mathcal{P}(s_1, s_2, \dots, s_T | \boldsymbol{\xi}_1, \boldsymbol{\xi}_2, \dots, \boldsymbol{\xi}_T)$

Intermediary variables that we will require in HMM

How to estimate the parameters of an HMM?

 \rightarrow Maximum of expected complete data log-likelihood $\mathcal{Q}(\Theta, \Theta^{\text{old}})$

How to compute
$$\frac{\partial Q}{\partial \Pi_i} = 0$$
, $\frac{\partial Q}{\partial a_{i,j}} = 0$, $\frac{\partial Q}{\partial \mu_i} = 0$ and $\frac{\partial Q}{\partial \Sigma_i} = 0$?

- \rightarrow Requires to compute $\zeta_{t,i,j}^{\text{HMM}} = \mathcal{P}(s_t = i, s_{t+1} = j \mid \boldsymbol{\xi}_{1:T})$
- \rightarrow Requires to compute $\gamma_{t,i}^{\text{\tiny HMM}} = \mathcal{P}(s_t = i \mid \boldsymbol{\xi}_{1:T})$

How to compute $\zeta_{t,i,j}^{\text{mm}}$ and $\gamma_{t,i}^{\text{mm}}$?

- \rightarrow Requires to compute $\alpha_{t,i}^{\text{HMM}} = \mathcal{P}(s_t = i, \boldsymbol{\xi}_{1:t})$
- \rightarrow Requires to compute $\beta_{t,i}^{\text{HMM}} = \mathcal{P}(\boldsymbol{\xi}_{t+1:T} \mid s_t = i)$







EM for HMM (Baum-Welch algorithm) E-step: compute $\gamma_{m,t,i}^{\text{HMM}}$ and $\zeta_{m,t,i,j}^{\text{HMM}}$ V1 V1 M-step: V2 V₂ $\Pi_i \leftarrow \frac{\sum_{m=1}^M \gamma_{m,1,i}^{\text{HMM}}}{M} = \frac{\text{Total number of times}}{\text{Total number of trajectories}}$ V٦ V3 Total number of $a_{i,j} \leftarrow \frac{\sum_{m=1}^{M} \sum_{t=1}^{T_{m-1}} \zeta_{m,t,i,j}^{\text{HMM}}}{\sum_{m=1}^{M} \sum_{t=1}^{T_{m-1}} \gamma^{\text{HMM}}} = \frac{\text{transitions from i to j}}{\text{Total number of times in i}}$ (and transit to anything else) $\boldsymbol{\mu}_{i} \leftarrow \frac{\sum_{m=1}^{M} \sum_{t=1}^{T_{m}} \gamma_{m,t,i}^{\text{HMM}} \boldsymbol{\xi}_{m,t}}{\sum_{m=1}^{M} \sum_{t=1}^{T_{m}} \gamma_{m,t,i}^{\text{HMM}}} \qquad \text{result similar to GMM}$ $\boldsymbol{\Sigma}_{i} \leftarrow \frac{\sum_{m=1}^{M} \sum_{t=1}^{T_{m}} \gamma_{m,t,i}^{\text{HMM}} \left(\boldsymbol{\xi}_{m,t} - \boldsymbol{\mu}_{i}\right) \left(\boldsymbol{\xi}_{m,t} - \boldsymbol{\mu}_{i}\right)^{\text{T}}}{\sum_{m=1}^{M} \sum_{t=1}^{T_{m}} \gamma_{m,t,i}^{\text{HMM}}}$

K Gaussians M sequences T_m points per sequences

The update rules can be interpreted as normalized counts, with several types of weighted averages required in the computation.

$$\begin{split} &\alpha_{t,i}^{\text{HMM}} = \mathcal{P}(s_t \!=\! i, \boldsymbol{\xi}_{1:t}) \\ &\beta_{t,i}^{\text{HMM}} = \mathcal{P}(\boldsymbol{\xi}_{t+1:T} \mid s_t \!=\! i) \\ &\gamma_{t,i}^{\text{HMM}} = \mathcal{P}(s_t \!=\! i \mid \boldsymbol{\xi}_{1:T}) \\ &\zeta_{t,i,j}^{\text{HMM}} \!=\! \mathcal{P}(s_t \!=\! i, s_{t\!+\!1} \!=\! j \mid \! \boldsymbol{\xi}_{1:T}) \end{split}$$

Useful intermediary variables in HMM

Forward variable
$$\alpha_{t,i}^{\text{HMM}} = \mathcal{P}(s_t = i, \boldsymbol{\xi}_{1:t})$$

 $\rho_{t,i} = \mathcal{P}(\boldsymbol{\xi}_{t+1:T} \mid \boldsymbol{s}_t = i)$ Backward variable

Smoothed node marginals

$$\gamma_{t,i}^{\text{\tiny HMM}} = \mathcal{P}(s_t = i \mid \boldsymbol{\xi}_{1:T})$$

Smoothed edge marginals

$$\zeta_{t,i,j}^{\text{mm}} = \mathcal{P}(s_t = i, s_{t+1} = j \mid \xi_{1:T})$$

Forward algorithm

 $\alpha_{t,i}^{\text{\tiny HMM}} = \mathcal{P}(s_t \!=\! i, \boldsymbol{\xi}_{1:t})$

The probability to be in state *i* at time step *t* and to observe $\boldsymbol{\xi}_{1:t} = \{ \boldsymbol{\xi}_1, \boldsymbol{\xi}_2, \dots, \boldsymbol{\xi}_t \}$ can be computed with the **forward variable**

$$\alpha_{t,i}^{\text{\tiny HMM}} = \mathcal{P}(s_t = i, \boldsymbol{\xi}_1, \boldsymbol{\xi}_2, \dots, \boldsymbol{\xi}_t) = \mathcal{P}(s_t = i, \boldsymbol{\xi}_{1:t})$$

which can be used to compute

$$\mathcal{P}(s_t = i \mid \boldsymbol{\xi}_{1:t}) = \frac{\mathcal{P}(s_t = i, \boldsymbol{\xi}_{1:t})}{\mathcal{P}(\boldsymbol{\xi}_{1:t})} = \frac{\alpha_{t,i}^{\text{HMM}}}{\sum_{k=1}^{K} \alpha_{t,k}^{\text{HMM}}}$$

The direct computation would require marginalizing over all possible state sequences $\{s_1, s_2, \ldots, s_{t-1}\}$, which would grow exponentially with t.

The forward algorithm takes advantage of the conditional independence rules of the HMM to perform the calculation recursively.





$$\alpha_{t,i}^{\text{\tiny HMM}} = \left(\sum_{j=1}^{K} \alpha_{t-1,j}^{\text{\tiny HMM}} a_{j,i}\right) \mathcal{N}(\boldsymbol{\xi}_t \mid \boldsymbol{\mu}_i, \boldsymbol{\Sigma}_i) \quad \text{with} \quad \alpha_{1,i}^{\text{\tiny HMM}} = \Pi_i \, \mathcal{N}(\boldsymbol{\xi}_1 \mid \boldsymbol{\mu}_i, \boldsymbol{\Sigma}_i)$$





It can be used to evaluate trajectories by computing the likelihood

 $\alpha_{t,i}^{\text{\tiny HMM}} = \mathcal{P}(s_t \!=\! i, \boldsymbol{\xi}_{1:t})$

$$\mathcal{P}(\boldsymbol{\xi} \,|\, \boldsymbol{\Theta}^{\text{mm}}) = \sum_{i=1}^{K} \alpha_{T,i}^{\text{mm}}$$

Useful intermediary variables in HMM

Forward variable
$$\alpha_{t,i}^{\text{\tiny HMM}} = \mathcal{P}(s_t = i, \boldsymbol{\xi}_{1:t})$$

Backward variable
$$eta_{t,i}^{\scriptscriptstyle ext{mm}} = \mathcal{P}(oldsymbol{\xi}_{t+1:T} \mid s_t \!=\! i)$$

Smoothed node marginals $\gamma_{t,i}^{\scriptscriptstyle ext{mm}} = \mathcal{P}(s_t)$

$$\gamma_{t,i}^{\text{\tiny HMM}} = \mathcal{P}(s_t = i \mid \boldsymbol{\xi}_{1:T})$$

Smoothed edge marginals $\zeta_{t,x}^{\text{\tiny HN}}$

$$\zeta_{t,i,j}^{\text{mm}} = \mathcal{P}(s_t = i, s_{t+1} = j \mid \boldsymbol{\xi}_{1:T})$$

$$\beta_{t,i}^{\text{\tiny HMM}} = \mathcal{P}(\boldsymbol{\xi}_{t+1:T} \mid s_t \!=\! i)$$

Similarly, we can define a **backward variable** starting from the boundary condition

 $\beta_{T,i}^{\mathrm{HMM}} = 1$

and computed as

$$\beta_{t,i}^{\text{HMM}} = \sum_{j=1}^{K} a_{i,j} \mathcal{N}(\boldsymbol{\xi}_{t+1} | \boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j) \beta_{t+1,j}^{\text{HMM}}$$

corresponding to the probability of the partial observation $\{\boldsymbol{\xi}_{t+1}, \ldots, \boldsymbol{\xi}_{T-1}, \boldsymbol{\xi}_T\}$, knowing that we are in state *i* at time step *t*.



Useful intermediary variables in HMM

These variable are sometimes called **smoothed variables** as they combine forward and backward probabilities in the computation.

You can think of their roles as passing "messages" from left to right, and from right to left, and then combining the information at each node.

Backward variable

Forward variable

$$eta_{t,i}^{\scriptscriptstyle ext{mmm}} = \mathcal{P}(oldsymbol{\xi}_{t-} \mid s_{t-})$$

 $lpha_{t.i}^{\scriptscriptstyle ext{mm}}=\mathcal{F}$

Smoothed node marginals $\gamma_{t,i}^{\scriptscriptstyle \mathrm{HMM}} =$

$$\boldsymbol{\mathcal{F}}_{t,i}^{\scriptscriptstyle \mathrm{HMM}} = \mathcal{P}(s_t \!=\! i \,|\, \boldsymbol{\xi}_{1:T})$$

Smoothed edge marginals

$$\zeta_{t,i,j}^{\text{mmm}} = \mathcal{P}(s_t = i, s_{t+1} = j \mid \boldsymbol{\xi}_{1:T})$$

Smoothed node marginals

$$\gamma_{t,i}^{\text{HMM}} = \frac{\alpha_{t,i}^{\text{HMM}} \ \beta_{t,i}^{\text{HMM}}}{\sum\limits_{k=1}^{K} \alpha_{t,k}^{\text{HMM}} \ \beta_{t,k}^{\text{HMM}}} = \frac{\alpha_{t,i}^{\text{HMM}} \ \beta_{t,i}^{\text{HMM}}}{\mathcal{P}(\boldsymbol{\xi})}$$

Useful intermediary variables in HMM

Forward variable
$$\alpha_{t,i}^{\text{\tiny HMM}} = \mathcal{P}(s_t = i, \boldsymbol{\xi}_{1:t})$$

Backward variable $\beta_{t,i}^{\text{HMM}} = \mathcal{P}(\boldsymbol{\xi}_{t+1:T} \mid s_t = i)$

Smoothed node marginals $\gamma_{t,i}^{\text{\tiny HMM}} = \mathcal{P}(s_t = i \mid \boldsymbol{\xi}_{1:T})$

Smoothed edge marginals $\zeta_{t,i,j}^{\text{\tiny HMM}} = \mathcal{P}(s_t = i, s_{t+1} = j | \boldsymbol{\xi}_{1:T})$

Smoothed edge marginals

$$\begin{split} \zeta_{t,i,j}^{\text{\tiny HMM}} &= \frac{\alpha_{t,i}^{\text{\tiny HMM}} \; a_{i,j} \; \mathcal{N}\big(\boldsymbol{\xi}_{t+1} | \; \boldsymbol{\mu}_{j}, \boldsymbol{\Sigma}_{j}\big) \; \beta_{t+1,j}^{\text{\tiny HMM}}}{\sum_{k=1}^{K} \sum_{l=1}^{K} \alpha_{t,k}^{\text{\tiny HMM}} \; a_{k,l} \; \mathcal{N}\big(\boldsymbol{\xi}_{t+1} | \; \boldsymbol{\mu}_{l}, \boldsymbol{\Sigma}_{l}\big) \; \beta_{t+1,l}^{\text{\tiny HMM}}} \\ &= \frac{\alpha_{t,i}^{\text{\tiny HMM}} \; a_{i,j} \; \mathcal{N}\big(\boldsymbol{\xi}_{t+1} | \; \boldsymbol{\mu}_{j}, \boldsymbol{\Sigma}_{j}\big) \; \beta_{t+1,j}^{\text{\tiny HMM}}}{\mathcal{P}(\boldsymbol{\xi})} \end{split}$$

EM for HMM (Baum-Welch algorithm) E-step: compute $\gamma_{m,t,i}^{\text{HMM}}$ and $\zeta_{m,t,i,j}^{\text{HMM}}$ V1 V1 M-step: V2 V₂ $\Pi_i \leftarrow \frac{\sum_{m=1}^M \gamma_{m,1,i}^{\text{HMM}}}{M} = \frac{\text{Total number of times}}{\text{Total number of trajectories}}$ V٦ V3 Total number of $a_{i,j} \leftarrow \frac{\sum_{m=1}^{M} \sum_{t=1}^{T_{m-1}} \zeta_{m,t,i,j}^{\text{HMM}}}{\sum_{m=1}^{M} \sum_{t=1}^{T_{m-1}} \gamma^{\text{HMM}}} = \frac{\text{transitions from i to j}}{\text{Total number of times in i}}$ (and transit to anything else) $\boldsymbol{\mu}_{i} \leftarrow \frac{\sum_{m=1}^{M} \sum_{t=1}^{T_{m}} \gamma_{m,t,i}^{\text{HMM}} \boldsymbol{\xi}_{m,t}}{\sum_{m=1}^{M} \sum_{t=1}^{T_{m}} \gamma_{m,t,i}^{\text{HMM}}} \qquad \text{result similar to GMM}$ $\boldsymbol{\Sigma}_{i} \leftarrow \frac{\sum_{m=1}^{M} \sum_{t=1}^{T_{m}} \gamma_{m,t,i}^{\text{HMM}} \left(\boldsymbol{\xi}_{m,t} - \boldsymbol{\mu}_{i}\right) \left(\boldsymbol{\xi}_{m,t} - \boldsymbol{\mu}_{i}\right)^{\text{T}}}{\sum_{m=1}^{M} \sum_{t=1}^{T_{m}} \gamma_{m,t,i}^{\text{HMM}}}$

K Gaussians M sequences Tm points per sequences

The update rules can be interpreted as normalized counts, with several types of weighted averages required in the computation.

$$egin{aligned} &lpha_{t,i}^{\scriptscriptstyle ext{\tiny HMM}} = \mathcal{P}(s_t\!=\!i,oldsymbol{\xi}_{1:t}) \ η_{t,i}^{\scriptscriptstyle ext{\tiny HMM}} = \mathcal{P}(oldsymbol{\xi}_{t+1:T} \mid s_t\!=\!i) \ η_{t,i}^{\scriptscriptstyle ext{\tiny HMM}} = \mathcal{P}(s_t\!=\!i \mid oldsymbol{\xi}_{1:T}) \ η_{t,i,j}^{\scriptscriptstyle ext{\tiny HMM}} = \mathcal{P}(s_t\!=\!i,s_{t\!+\!1}\!=\!j |oldsymbol{\xi}_{1:T}) \end{aligned}$$

For long sequences, the forward and backward variables can quickly get very low, likely exceeding the precision range of the computer.

A simple scaling procedure is to multiply $\alpha_{t,i}^{\text{\tiny HMM}}$ by a factor independent of i, and divide $\beta_{t,i}^{\text{\tiny HMM}}$ by the same factor so that they are cancelled in the forward-backward computation.

The computation can be kept within reasonable bounds by setting the scaling factor

$$c_t = \frac{1}{\sum_{i=1}^{K} \alpha_{t,i}^{\mathrm{HMM}}}$$

Numerical underflow issue in HMM

 $c_t = \frac{1}{\sum_{i=1}^{K} \alpha_{t,i}^{\mathrm{HMM}}}$

This issue is sometimes not covered in textbooks, although it remains very important for practical implementation of HMM!

We have by induction

$$\hat{\alpha}_{t,i}^{\text{HMM}} = \left(\prod_{s=1}^{t} c_s\right) \alpha_{t,i}^{\text{HMM}} , \quad \hat{\beta}_{t,i}^{\text{HMM}} = \left(\prod_{s=t}^{T} c_s\right) \beta_{t,i}^{\text{HMM}}$$

With this, the numerator and denominator will cancel out when used in the re-estimation formulas. For example

$$\gamma_{t,i}^{\text{HMM}} = \frac{\hat{\alpha}_{t,i}^{\text{HMM}} \hat{\beta}_{t,i}^{\text{HMM}}}{\sum\limits_{k=1}^{K} \hat{\alpha}_{t,k}^{\text{HMM}} \hat{\beta}_{t,k}^{\text{HMM}}} = \frac{\left(\prod_{s=1}^{t} c_{s}\right) \left(\prod_{s=t}^{T} c_{s}\right) \alpha_{t,i}^{\text{HMM}} \beta_{t,i}^{\text{HMM}}}{\left(\prod_{s=1}^{t} c_{s}\right) \left(\prod_{s=t}^{T} c_{s}\right) \sum\limits_{k=1}^{K} \alpha_{t,k}^{\text{HMM}} \beta_{t,k}^{\text{HMM}}}} = \frac{\alpha_{t,i}^{\text{HMM}} \beta_{t,i}^{\text{HMM}}}{\sum\limits_{k=1}^{K} \alpha_{t,k}^{\text{HMM}} \beta_{t,k}^{\text{HMM}}}$$

Why did we introduce these intermediary variables in HMM?

Forward variable $\alpha_{t,i}^{\text{\tiny HMM}} = \mathcal{P}(s_t = i, \boldsymbol{\xi}_{1:t})$

Backward variable $\beta_{t,i}^{\text{\tiny HMM}} = \mathcal{P}(\boldsymbol{\xi}_{t+1:T} \mid s_t \!=\! i)$

Smoothed node marginals $\gamma_{t,i}^{\scriptscriptstyle \mathrm{HMM}} = \mathcal{P}(s_t \!=\! i \,|\, \boldsymbol{\xi}_{1:T})$

Smoothed edge marginals $\zeta_{t,i,j}^{\text{\tiny HMM}} = \mathcal{P}(s_t = i, s_{t+1} = j \mid \boldsymbol{\xi}_{1:T})$

Why did we introduce these intermediary variables in HMM?

How to estimate the parameters of an HMM?

 \rightarrow Maximum of expected complete data log-likelihood $\mathcal{Q}(\Theta, \Theta^{\text{old}})$

How to compute
$$\frac{\partial Q}{\partial \Pi_i} = 0$$
, $\frac{\partial Q}{\partial a_{i,j}} = 0$, $\frac{\partial Q}{\partial \mu_i} = 0$ and $\frac{\partial Q}{\partial \Sigma_i} = 0$?

- \rightarrow Requires to compute $\zeta_{t,i,j}^{\text{HMM}} = \mathcal{P}(s_t = i, s_{t+1} = j \mid \boldsymbol{\xi}_{1:T})$
- \rightarrow Requires to compute $\gamma_{t,i}^{\text{\tiny HMM}} = \mathcal{P}(s_t = i \mid \boldsymbol{\xi}_{1:T})$

How to compute $\zeta_{t,i,j}^{\text{mm}}$ and $\gamma_{t,i}^{\text{mm}}$?

- \rightarrow Requires to compute $\alpha_{t,i}^{\text{HMM}} = \mathcal{P}(s_t = i, \boldsymbol{\xi}_{1:t})$
- \rightarrow Requires to compute $\beta_{t,i}^{\text{HMM}} = \mathcal{P}(\boldsymbol{\xi}_{t+1:T} \mid s_t = i)$

Observations $\boldsymbol{\xi}_{1:T}$

Viterbi decoding (MAP vs MPE estimates) Maximum a posteriori Most probable explanation

Python notebook: demo_HMM.ipynb

Matlab code: demo_HMM_Viterbi01.m

The (jointly) most probable sequence of states $\hat{\boldsymbol{s}}^{\text{MAP}}$ is not necessarily the same as the sequence of (marginally) most probable states $\hat{\boldsymbol{s}}^{\text{MPE}}$

$$\hat{\boldsymbol{s}}^{\text{MAP}} = \underset{\{s_1, s_2, \dots, s_T\}}{\operatorname{arg max}} \mathcal{P}(\boldsymbol{s} | \boldsymbol{\xi})$$

$$\hat{\boldsymbol{s}}^{\text{MAP}} = \left\{ \arg \max_{s_1} \underbrace{\mathcal{P}(s_1 | \boldsymbol{\xi})}_{r_1}, \arg \max_{s_2} \underbrace{\mathcal{P}(s_2 | \boldsymbol{\xi})}_{r_2}, \dots, \arg \max_{s_T} \underbrace{\mathcal{P}(s_T | \boldsymbol{\xi})}_{r_1} \right\}$$

 \hat{s}^{MAP} can be computed with the **Viterbi algorithm**, employing the max operator in a forward pass, followed by a backward pass using a **fast traceback procedure** to recover the most probable path.

Viterbi decoding

states j that maximized $\delta_{t,i}$.

Backtracking: S

$$\hat{s}_t^{\text{map}} = \Psi_{t+1, \, \hat{s}_{t+1}^{\text{map}}}$$

Viterbi decoding - Example

$$\delta_{t,i} = \max_{j} (\delta_{t-1,j} \ a_{j,i}) \ b(\boldsymbol{\xi}_{t}|i)$$

with $\delta_{1,i} = \prod_{i} \mathcal{N}(\boldsymbol{\xi}_{1}| \ \boldsymbol{\mu}_{i}, \boldsymbol{\Sigma}_{i})$

Observation: $\boldsymbol{\xi} = \{C1, C3, C4, C6\}$

Numerical underflow issue in Viterbi

Similarly to the forward-backward variables in HMM, we have to take care about potential numerical underflow when implementing Viterbi decoding.

A simple way is to normalize $\delta_{t,i}$ at each time step t by multiplying it with

$$c_t = \frac{1}{\sum_{i=1}^K \delta_{t,i}}$$

similarly as in the computation of the forward-backward variables. Such scaling will not affect the maximum.

Numerical underflow issue in Viterbi

Alternatively, we can work in the log domain. We then have

$$\log \delta_{t,i} = \max_{\boldsymbol{s}_{1:t-1}} \log \mathcal{P}(\boldsymbol{s}_{1:t-1}, \boldsymbol{s}_t = i | \boldsymbol{\xi}_{1:t}) = \max_{j} \left(\log \delta_{t-1,j} + \log a_{i,j} \right) + \log \mathcal{N}(\boldsymbol{\xi}_t | \boldsymbol{\mu}_i, \boldsymbol{\Sigma}_i)$$

With high dimensional Gaussians as emission distributions, the Viterbi computation with log can result in a **significant speedup**, since computing $\log \mathcal{P}(\boldsymbol{\xi}_t | s_t)$ can be much faster than computing $\mathcal{P}(\boldsymbol{\xi}_t | s_t)$.

When training HMMs, the Viterbi algorithm can be also used (instead of the forward-backward variables) in the E step of the EM procedure.

Hidden semi-Markov model (HSMM)

> Python notebook: demo_HSMM.ipynb

Matlab code: demo_HSMM01.m

State duration probability in standard HMM

The state duration follows a geometric distribution

$$\mathcal{P}(d) = a_{i,i}^{d-1}(1 - a_{i,i})$$

Naive approach: By artificially duplicating the number of states while keeping the same emission distribution, other state duration distributions can be modeled

Hidden semi-Markov model (HSMM)

Hidden semi-Markov model (HSMM)

HMM with dynamic features (Trajectory-HMM)

Matlab code: demo_trajHSMM01.m

For the encoding of movements, velocity and acceleration can be used as dynamic features. By considering an Euler approximation, the velocity is computed as

$$\dot{oldsymbol{x}}_t = rac{oldsymbol{x}_{t+1} - oldsymbol{x}_t}{\Delta t}$$

where \boldsymbol{x}_t is a multivariate position vector.

The acceleration is similarly computed as

$$\ddot{\boldsymbol{x}}_t = \frac{\dot{\boldsymbol{x}}_{t+1} - \dot{\boldsymbol{x}}_t}{\Delta t} = \frac{\boldsymbol{x}_{t+2} - 2\boldsymbol{x}_{t+1} + \boldsymbol{x}_t}{\Delta t^2}$$

$$\dot{\boldsymbol{x}}_t = \frac{\boldsymbol{x}_{t+1} - \boldsymbol{x}_t}{\Delta t}, \quad \ddot{\boldsymbol{x}}_t = \frac{\boldsymbol{x}_{t+2} - 2\boldsymbol{x}_{t+1} + \boldsymbol{x}_t}{\Delta t^2}$$

A vector $\boldsymbol{\zeta}_t$ will be used to represent the concatenated position, velocity and acceleration vectors at time step t

$$oldsymbol{\zeta}_t = egin{bmatrix} oldsymbol{x}_t \ \dot{oldsymbol{x}}_t \ \ddot{oldsymbol{x}}_t \end{bmatrix} = egin{bmatrix} oldsymbol{I} & oldsymbol{0} & oldsymbol{0} & oldsymbol{0} & oldsymbol{0} & oldsymbol{x}_t \ -rac{1}{\Delta t}oldsymbol{I} & oldsymbol{1} & oldsymbol{0} & oldsymbol{0} & oldsymbol{0} & oldsymbol{x}_t \ rac{1}{\Delta t^2}oldsymbol{I} & oldsymbol{-} & oldsymbol{0} & oldsymbol{0} & oldsymbol{0} & oldsymbol{0} & oldsymbol{x}_t \ oldsymbol{x}_{t+1} & oldsymbol{0} & oldsymbol{0} & oldsymbol{x}_{t+1} \ rac{1}{\Delta t^2}oldsymbol{I} & oldsymbol{-} & oldsymbol{1} & oldsymbol{1} & oldsymbol{x}_{t+1} \ oldsymbol{x}_{t+2} \end{bmatrix} egin{matrix} oldsymbol{x}_t & oldsymbol{1} & oldsymbol{0} & oldsymbol{0} & oldsymbol{x}_{t+1} \ oldsymbol{x}_{t+2} \end{bmatrix} egin{matrix} oldsymbol{x}_t & oldsymbol{1} & oldsymbol{1} & oldsymbol{1} & oldsymbol{x}_{t+1} \ oldsymbol{x}_{t+2} \end{bmatrix} egin{matrix} oldsymbol{x}_t & oldsymbol{1} & oldsymbol{0} & oldsymbol{1} & oldsymbol{x}_{t+1} \ oldsymbol{x}_{t+2} \end{bmatrix} egin{matrix} oldsymbol{x}_t & oldsymbol{1} & oldsymbol{1} & oldsymbol{1} & oldsymbol{x}_{t+1} \ oldsymbol{x}_{t+2} \end{bmatrix} egin{matrix} oldsymbol{1} & oldsymbo$$

Here, the number of derivatives will be set up to acceleration (C=3), but the same approach can be applied to a different number of derivatives.

A GMM/HMM/HSMM with centers $\{\boldsymbol{\mu}_i\}_{i=1}^K$ and covariance matrices $\{\boldsymbol{\Sigma}_i\}_{i=1}^K$ is first fit to the dataset $[\boldsymbol{\zeta}_1, \boldsymbol{\zeta}_2, \dots, \boldsymbol{\zeta}_T]$.

 $oldsymbol{\zeta}_t = egin{bmatrix} oldsymbol{x}_t \ \dot{oldsymbol{x}}_t \ \dot{oldsymbol{x}}_t \end{bmatrix}$

 $\pmb{\zeta}$ and \pmb{x} are defined as large vectors concatenating $\pmb{\zeta}_t$ and \pmb{x}_t for all time steps

$$oldsymbol{\zeta} = egin{bmatrix} oldsymbol{\zeta}_1 \ oldsymbol{\zeta}_2 \ dots \ oldsymbol{\zeta}_T \end{bmatrix} egin{matrix} oldsymbol{x} = egin{bmatrix} oldsymbol{x}_1 \ oldsymbol{x}_2 \ dots \ oldsymbol{z}_2 \ dots \ oldsymbol{z}_2 \ dots \ oldsymbol{z}_T \end{bmatrix} egin{matrix} oldsymbol{x} = egin{matrix} oldsymbol{x}_1 \ oldsymbol{x}_2 \ dots \ dots \ oldsymbol{z}_2 \ dots \ dots \ oldsymbol{x}_T \end{bmatrix} egin{matrix} oldsymbol{x} = egin{matrix} oldsymbol{x}_1 \ oldsymbol{x}_2 \ dots \ dots \ dots \ oldsymbol{x}_T \end{bmatrix} egin{matrix} oldsymbol{x} = egin{matrix} oldsymbol{x}_1 \ oldsymbol{x}_2 \ dots \ dots \ oldsymbol{x}_T \end{bmatrix} egin{matrix} oldsymbol{x} = egin{matrix} oldsymbol{x}_1 \ oldsymbol{x}_2 \ dots \ dots \ oldsymbol{x}_T \end{bmatrix} egin{matrix} oldsymbol{x} = egin{matrix} oldsymbol{x}_1 \ oldsymbol{x}_2 \ dots \ dots \ oldsymbol{x}_T \end{bmatrix} egin{matrix} oldsymbol{x} = egin{matrix} oldsymbol{x}_1 \ oldsymbol{x}_2 \ dots \ dots \ oldsymbol{x}_T \end{bmatrix} egin{matrix} oldsymbol{x} = egin{matrix} oldsymbol{x}_1 \ oldsymbol{x}_2 \ dots \ dots \ oldsymbol{x}_T \end{bmatrix} egin{matrix} oldsymbol{x} = egin{matrix} oldsymbol{x} \ dots \ dot$$

Similarly to the matrix operator defined in the previous slide for a single time step, a large sparse matrix Φ can be defined so that

$$oldsymbol{\zeta} = \Phi x$$

D dimensions*C* derivatives*T* time steps

By providing explicitly a sequence of states $\boldsymbol{s} = \{s_1, s_2, \ldots, s_T\}$ of T time steps (e.g., retrieved by Viterbi or specified manually), with discrete states $s_t \in \{1, \ldots, K\}$, the likelihood of a movement $\boldsymbol{\zeta} = \boldsymbol{\Phi} \boldsymbol{x}$ is given by

$$\mathcal{P}(oldsymbol{\zeta}|oldsymbol{s}) = \prod_{t=1}^{-} \mathcal{N}(oldsymbol{\zeta}_t \,|\, oldsymbol{\mu}_{s_t}, oldsymbol{\Sigma}_{s_t})$$

where $\boldsymbol{\mu}_{s_t}$ and $\boldsymbol{\Sigma}_{s_t}$ are the center and covariance of state s_t at time step t.

This product can be rewritten as

$$\mathcal{P}(\boldsymbol{\zeta}|\boldsymbol{s}) = \mathcal{N}(\boldsymbol{\zeta} \mid \boldsymbol{\mu}_{\boldsymbol{s}}, \boldsymbol{\Sigma}_{\boldsymbol{s}})$$
with $\boldsymbol{\mu}_{\boldsymbol{s}} = \begin{bmatrix} \boldsymbol{\mu}_{s_1} \\ \boldsymbol{\mu}_{s_2} \\ \vdots \\ \boldsymbol{\mu}_{s_T} \end{bmatrix}$ and $\boldsymbol{\Sigma}_{\boldsymbol{s}} = \begin{bmatrix} \boldsymbol{\Sigma}_{s_1} & \boldsymbol{0} & \cdots & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{\Sigma}_{s_2} & \cdots & \boldsymbol{0} \\ \vdots & \vdots & \ddots & \vdots \\ \boldsymbol{0} & \boldsymbol{0} & \cdots & \boldsymbol{\Sigma}_{s_T} \end{bmatrix}$

For example, for a sequence of states $\mathbf{s} = \{1, 1, 2, 2, 3, 3, 3, 4\}$ with K=4 and T=8, we have

$\mu_s =$	$oxed{\mu}_1$			Σ_1	0	0	0	0	0	0	0
	$oldsymbol{\mu}_1$		$\Sigma_s =$	0	$\mathbf{\Sigma}_1$	0	0	0	0	0	0
	$oldsymbol{\mu}_2$			0	0	$\mathbf{\Sigma}_2$	0	0	0	0	0
	$oldsymbol{\mu}_2$	and		0	0	0	$\mathbf{\Sigma}_2$	0	0	0	0
	$oldsymbol{\mu}_3$	and		0	0	0	0	$\mathbf{\Sigma}_3$	0	0	0
	$oldsymbol{\mu}_3$			0	0	0	0	0	$\mathbf{\Sigma}_3$	0	0
	$oldsymbol{\mu}_3$			0	0	0	0	0	0	$\mathbf{\Sigma}_3$	0
	$oldsymbol{\mu}_4$			0	0	0	0	0	0	0	$\mathbf{\Sigma}_4$

 $oldsymbol{\mu}_{s} \in \mathbb{R}^{DCT}$

 $\boldsymbol{\Sigma_s} \in \mathbb{R}^{DCT imes DCT}$

By using the relation $\boldsymbol{\zeta} = \boldsymbol{\Phi} \boldsymbol{x}$, we want to retrieve a trajectory

$$\hat{\boldsymbol{x}} = \arg \max_{\boldsymbol{x}} \log \mathcal{P}(\boldsymbol{\Phi}\boldsymbol{x} \mid \boldsymbol{s})$$

$$\begin{pmatrix} \\ \\ \\ \mathcal{N}(\boldsymbol{\Phi}\boldsymbol{x} \mid \boldsymbol{\mu}_{s}, \boldsymbol{\Sigma}_{s}) = (2\pi)^{-\frac{DCT}{2}} |\boldsymbol{\Sigma}_{s}|^{-\frac{1}{2}} \exp\left(-\frac{1}{2}(\boldsymbol{\Phi}\boldsymbol{x} - \boldsymbol{\mu}_{s})^{\mathsf{T}} \boldsymbol{\Sigma}_{s}^{-1}(\boldsymbol{\Phi}\boldsymbol{x} - \boldsymbol{\mu}_{s})^{\mathsf{T}} \boldsymbol{\Sigma}_{s}^{\mathsf{T}} \boldsymbol{\Sigma}_{s}^{\mathsf{T}}$$

Equating to zero the derivative of

$$\log \mathcal{P}(\boldsymbol{\Phi}\boldsymbol{x} \mid \boldsymbol{s}) = -\frac{1}{2} (\boldsymbol{\Phi}\boldsymbol{x} - \boldsymbol{\mu}_{\boldsymbol{s}})^{\mathsf{T}} \boldsymbol{\Sigma}_{\boldsymbol{s}}^{-1} (\boldsymbol{\Phi}\boldsymbol{x} - \boldsymbol{\mu}_{\boldsymbol{s}}) - \frac{1}{2} \log |\boldsymbol{\Sigma}_{\boldsymbol{s}}| - \frac{DCT}{2} \log(2\pi)$$

with respect to \boldsymbol{x} yields

The residual error of this estimate is given by the covariance matrix

$$\mathbf{\hat{\Sigma}}^{m{x}} = \sigma ig(\mathbf{\Phi}^{\scriptscriptstyle op} \mathbf{\Sigma}_{m{s}}^{-1} \mathbf{\Phi} ig)^{-1}$$

where σ is a scaling factor.

The resulting Gaussian $\mathcal{N}(\hat{\boldsymbol{x}}, \hat{\boldsymbol{\Sigma}}^{\boldsymbol{x}})$ forms a trajectory distribution, where $\hat{\boldsymbol{x}} \in \mathbb{R}^{DT}$ is an average trajectory stored in a vector form.

HMM with dynamic features - Summary

 $\mathcal{N}(oldsymbol{\hat{x}}, oldsymbol{\hat{\Sigma}^{x}})$

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