Introduction to Machine Learning

Hidden Markov Models

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July 8, 2018

Outline

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Markov Random Processes

Markov process (First-Order Markov Model)

A stochastic process is called a Markov process when it has the Markov property:

$$P\left(X_{t_n}|X_{t_{n-1}}=x_{n-1},...X_{t_1}=x_1\right)=P\left(X_{t_n}|X_{t_{n-1}}=x_{n-1}\right) \quad (1)$$

Simply

The future path of a Markov process, given its current state and the past history before, depends only on the current state (not on how this state has been reached).

Thus (Quite an Oversimplification!!!)

A Markov process is characterized by the (one-step) transition probabilities:

$$p_{ij}=P\left(X_n=j|X_{n-1}=i\right) \quad (2)$$

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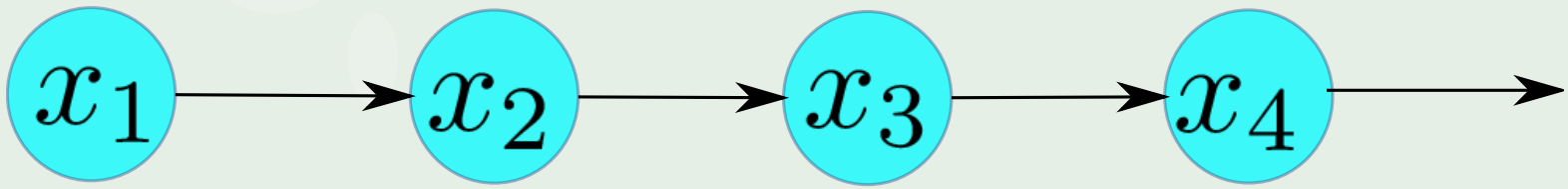
Graphical Interpretation

A sequence of events depending only in the previous one

$$P\left(x_n|x_{n-1}\right)$$



Markov Chains

Definition (Oversimplified)

A Markov chain is thus a process X_n indexed by integers $n = 0, 1, ...$ such that the states of the system are being indexed by integers $X_n = 0, 1, ...$

From here

The probability of a path $i_1, i_2, ..., i_n$ is

$$P(X_1 = i_1, X_2 = i_2, ..., X_n = i_n) = P(X_1 = i_1) p_{i_1 i_2} p_{i_2 i_3} \cdots p_{i_{n-1} i_n} \quad (3)$$

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The Transition Probability Matrix of a Markov chain

Thus

The transition probabilities can be arranged as transition probability matrix $\boldsymbol{P} = (p_{i,j})$

$$\text{Final State} \longrightarrow$$

$$\text{Initial State} \downarrow \begin{pmatrix} p_{1,1} & p_{1,2} & p_{1,3} & \cdots \\ p_{2,1} & p_{2,2} & p_{2,3} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} = \boldsymbol{P}$$

Propertities

The row i contains the transition probabilities from state i to other states.

- Since the system always goes to some state, the sum of the column probabilities is 1

Then

A matrix with non-negative elements such that the sum of each column equals 1 is called a stochastic matrix.

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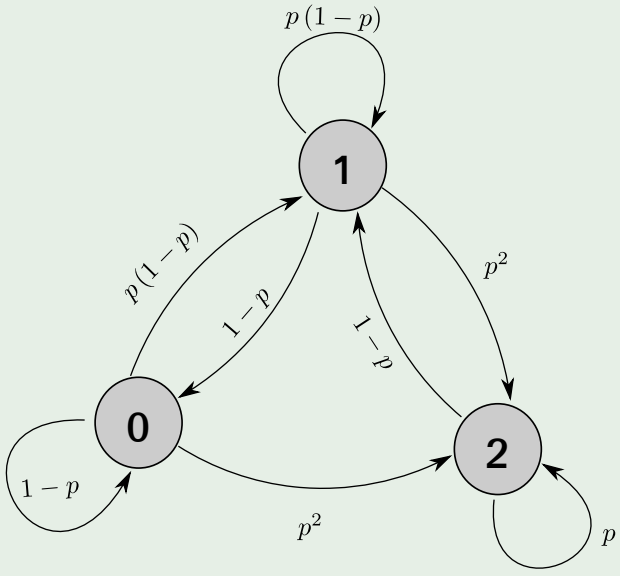
Example

We have the following state machine



We have the following Stochastic Matrix

$$M = \begin{pmatrix} 1-p & 1-p & 0 \\ p(1-p) & p(1-p) & 1-p \\ p^2 & p^2 & p \end{pmatrix} \tag{4}$$

With $p = \frac{1}{3}$

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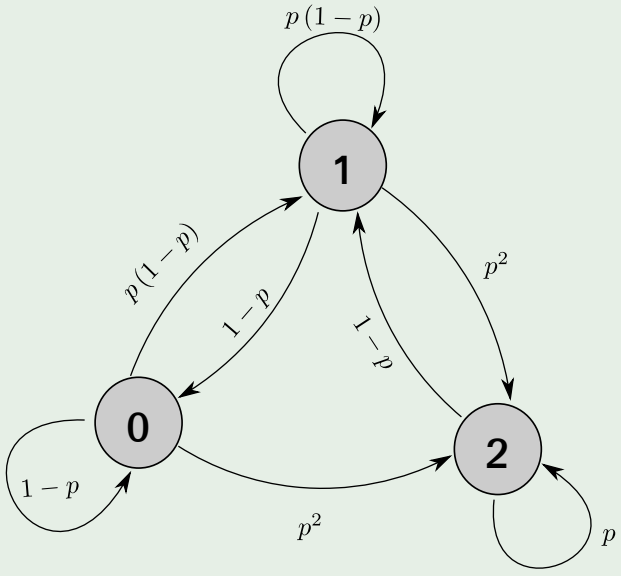

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Using this

We can talk about an initial distribution is given as a row vector π

A stationary probability vector π is defined as a distribution, written as a row vector, that does not change under application of the transition matrix:

$$\pi = P\pi \tag{5}$$

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Based in the Perron-Frobenious Theorem (Read about it in Wolfran-MathWorld)

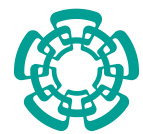
Theorem: Let M be a Markov chain whose left stochastic matrix has no zeros. Then, M has a single stationary distribution, and it converges to this when started at any distribution.

How to find the stationary distribution

We can find this stationary distribution using a slow process called the Power Method

There are others:

- Householder transformations
- Givens rotations
- Arnoldi iteration



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Class Sequence and Observations

We have

A sequence of T (feature vectors) observations, $X = \langle \boldsymbol{x}_1, \boldsymbol{x}_2, ..., \boldsymbol{x}_T \rangle$.

In addition

A collection of N classes or hidden states, $\omega_1, \omega_2, ..., \omega_N$

Thus, we have an element like this one

$$\Omega = \langle \omega_1, \omega_2, ..., \omega_T \rangle \tag{6}$$

Note: Total number of class sequences is N^T for sequences of size T.

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Transition Model

Definition of the transition model $\lambda = (A, B, \pi)$ for Hidden Markov Model (HMM)

Where:

1. N is the number of hidden states.
2. M is the number of different observation symbols.
3. $A = \{a_{ij}\}$is the stat transition probability $a_{ij} = P(q_{t+1} = \omega_j | q_t = \omega_i)$ with $1 \leq i, j \leq N$ (In our case $a_{ij} > 0$).
4. $B = \{b_j(x_k)\}$ is the observation symbol probability at state j i.e. $b_j(x_k) = P(x_k | q_t = \omega_j)$ such that $1 \leq j \leq N$ and $1 \leq k \leq M$.
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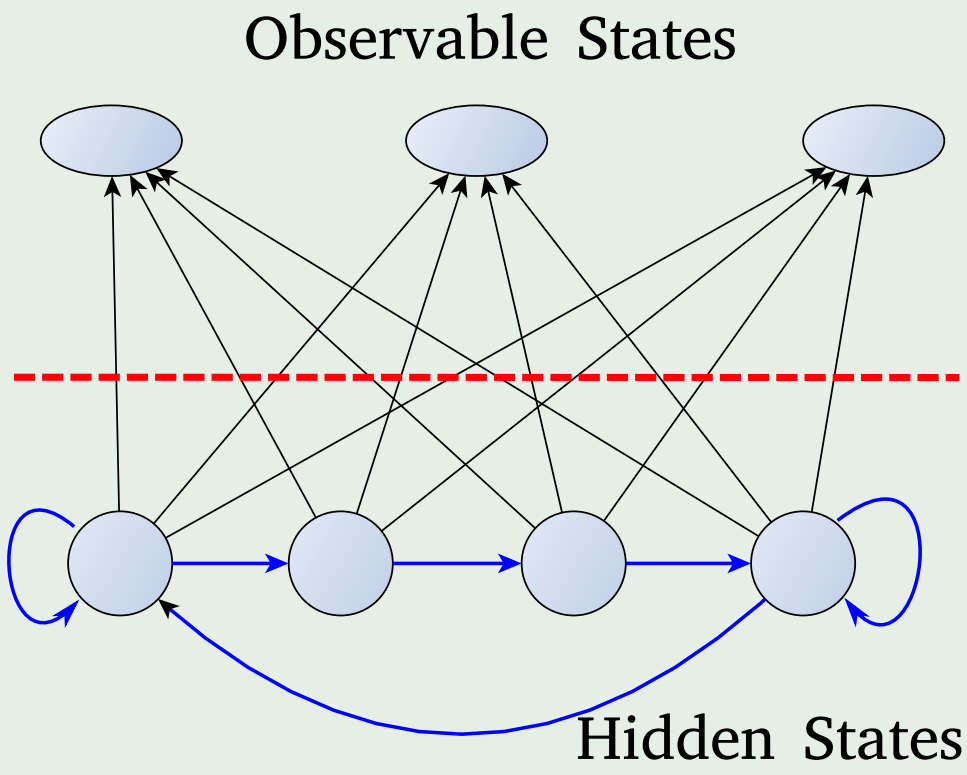
Example

We have that

The hidden states conform a probabilistic state machine with emission probability for the symbols.



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Using a HMM

It can be used as a generator of sequences X

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2. Set $t = 1$.
3. Choose an observation $X_t = x_k$ according to the symbol probability in state ω_i, $b_i(k)$.
4. Transit to a new state $q_{t+1} = \omega_j$ according to the state transition probability distribution for state ω_i, a_{ij}.
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How do we implement this

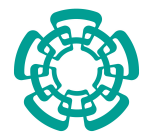
We need to move from q_i to q_{i+1}

- To move from one state to another it is possible to use the following algorithm

Roulette Wheel Selection

1. Allocate an array A of size $n+1$.
2. Set $A[1]=a_{i1}$.
3. For each probability a_{ij} from 1 to $n-1$:

$$A[j] = A[j-1] + p_j \text{ (Cumulative Probability)}$$



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1. Generate a uniformlyrandom value x in the range $[0, 1)$.
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What do we want?

Problem 1

Given the sequence X and a certain model λ, How we efficiently compute $P(X|\lambda)$?

Problem 2

Given the observation sequence X and a model λ, How we choose a corresponding class sequence Ω? Which best explains the observations.

Problem 3

How do we ajust the parameters of the λ to maximize $P(X|\lambda)$?

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Our task is to decide to which class sequence $\Omega = \langle \omega_1, \omega_2, ..., \omega_T \rangle$ the sequence $X = \langle \boldsymbol{x}_1, \boldsymbol{x}_2, ..., \boldsymbol{x}_T \rangle$ belongs.

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Given the sequence of classes, the observations are statistically independent.

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Using our notation

Then

$$P(\Omega|\lambda) = \pi_1 a_{1,2} \cdots a_{T-1,T} \tag{9}$$

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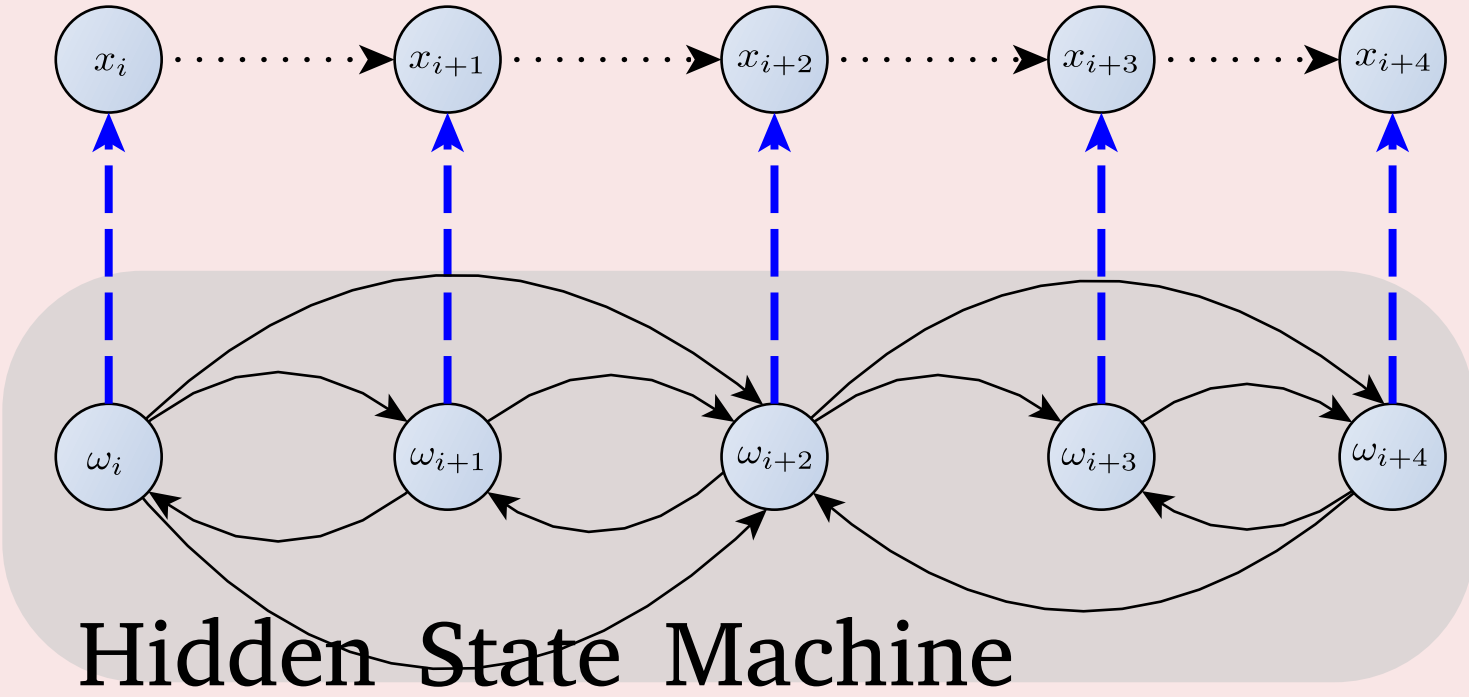
What do we want?

Then, we want to the probability of X and Ω to happen simultaneously

$$P(X, \Omega|\lambda) = P(X|\Omega, \lambda) P(\Omega|\lambda) \tag{11}$$



Outline

Thus, we need to calculate

What?

$$P(X|\lambda) = \sum_{\Omega} P(X, \Omega|\lambda) \tag{12}$$

Using Bayes Rule

$$P(X|\lambda) = \sum_{\Omega} P(X|\Omega, \lambda) P(\Omega|\lambda) \tag{13}$$

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Putting All Together

Thus, we have then

$$P(X|\lambda) = \sum_{\Omega} P(X|\Omega, \lambda) P(\Omega|\lambda)$$

$$= \sum_{q_1, q_2, \ldots, q_T} \pi_1 b_{q_1}(x_1) \left[a_{q_1,q_2} b_{q_2}(x_2)\right] \cdots \left[b_{q_T}(x_T)\right]$$

Putting All Together

Thus, we have then

$$P(X|\lambda) = \sum_{\Omega} P(X|\Omega,\lambda)\, P(\Omega|\lambda)$$
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Complexity for brute force approach

Multiplications

We need $2T$ multiplications (Rearranging):

$$\underbrace{\left[\pi_1 a_{q_1,q_2}\cdots a_{q_{T-1},q_T}\right]}_{T}\underbrace{\left[b_{q_1}\left(x_1\right)\cdots b_{q_T}\left(x_T\right)\right]}_{T} \tag{14}$$

Sums

We need N^T additions because of the term $\sum_{q_1,q_2,\cdots,q_T}$.

Total number of Operations

$$O\left(TN^T\right) \tag{15}$$

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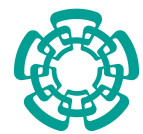
Outline

This will become part of a Dynamic Programming Solution

Together with a Backward procedure

The forward and backward procedure will help to solve the second problem

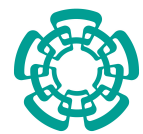


Consider the following

Define

$$\alpha_t(i) = P(x_1, x_2, ..., x_t, q_t = \omega_i | \lambda) \tag{16}$$

Probability of the partial observation until time t and state ω_i.



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We can use an induction, we need to prove

1. Initialization $\alpha_1(i) = \pi_i b_i(x_1)\ 1 \leq i \leq N$
2. Induction $\alpha_{t+1}(j) = \left[\sum_{i=1}^{N} \alpha_t(i) a_{ij}\right] b_j(O_{t+1})\ 1 \leq t \leq T-1$ and $1 \leq j \leq N$.
3. Termination $P(X|\lambda) = \sum_{i=1}^{N} \alpha_T(i)$

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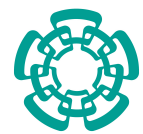

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Outline

How do we do this?

Step 1

You need to prove it is correct for $\alpha_1(i)$ with $1 \leq i \leq N$

Assume it is true for t

Then, you need to prove it for $\alpha_{t+1}(j)$ with $1 \leq t \leq T-1$ and $1 \leq j \leq N$.

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Initializes the forward probabilities as

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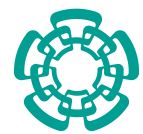
Here is the idea of moving from one state at time t to another state on time $t + 1$



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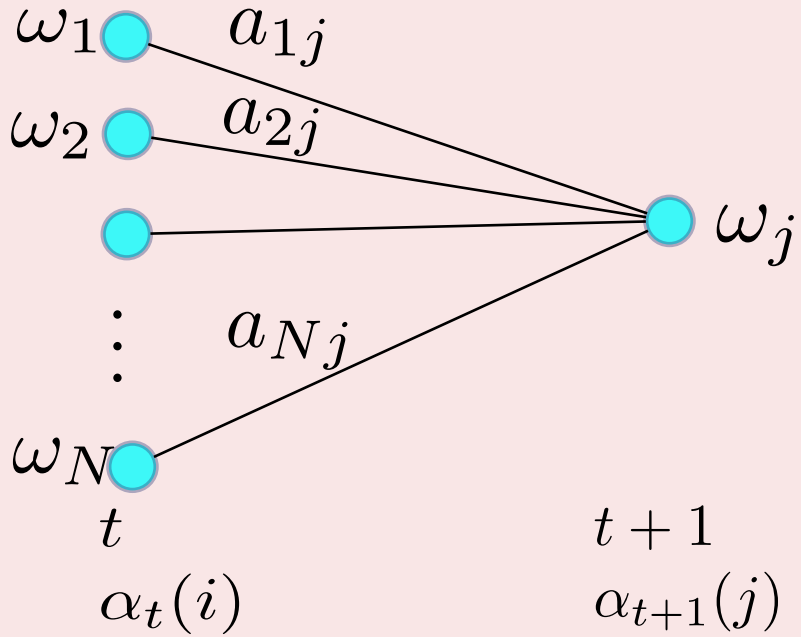
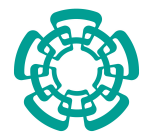


What?

Basically

Our problem is we do not now from which state we start to arrive to j

Now, we start calculate $\alpha_{t+1}(j)$



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$$= P(x_{t+1} | x_1, x_2, ..., x_t, q_{t+1} = \omega_j, \lambda) \times \cdots$$

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Our problem is we do not now from which state we start to arrive to j

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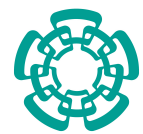
$$\begin{aligned}\alpha_{t+1}(j) =& P(x_1, x_2, ..., x_t, x_{t+1}, q_{t+1} = \omega_j|\lambda) \\ =& P(x_{t+1}|x_1, x_2, ..., x_t, q_{t+1} = \omega_j, \lambda) \times \cdots \\ & P(x_1, x_2, ..., x_t, q_{t+1} = \omega_j|\lambda)\end{aligned}$$



We need to calculate

First

$$P\left(x_{t+1}|x_1, x_2, ..., x_t, q_{t+1} = \omega_j, \lambda\right) \tag{18}$$

Second

$$P\left(x_1, x_2, ..., x_t, q_{t+1} = \omega_j|\lambda\right) \tag{19}$$

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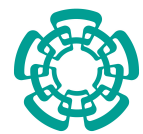
We have that

$$P(x_1, x_2, ..., x_t, q_{t+1} = \omega_j|\lambda) =$$

$$= \sum_{i=1}^{N} P(x_1, x_2, ..., x_t, q_t = \omega_i, q_{t+1} = \omega_j|\lambda)$$

The second step is due to applying the marginal formula over all possible states



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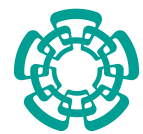

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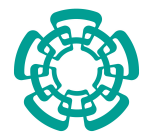

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Finally

This true for

$t = 1, 2, ..., T-1$ and $1 \leq j \leq N$.

Now, applying the marginal idea for $P(x_1, x_2, ..., x_T|\lambda)$

$$P(x_1, x_2, ..., x_T|\lambda) = \sum_{i=1}^{N} P(x_1, x_2, ..., x_T, q_T = \omega_i|\lambda) = \sum_{i=1}^{N} \alpha_T(i) \quad (23)$$

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Complexity

Given that we are requiered to compute the $\alpha_t(j)$

For $1 \leq t \leq T$ and $1 \leq j \leq N$

We can calculate this using a table (Dynamic Programming Idea)

t \ j	1	2	$\cdots$	N
1	$\alpha_1(1)$	$\alpha_1(2)$	$\cdots$	$\alpha_1(N)$
2	$\alpha_2(1)$	$\underbrace{\alpha_2(1)}_{\text{Cost } N}$	$\cdots$	$\alpha_2(N)$
$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$
T	$\alpha_T(1)$	$\alpha_T(2)$	$\cdots$	$\alpha_T(N)$

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Complexity

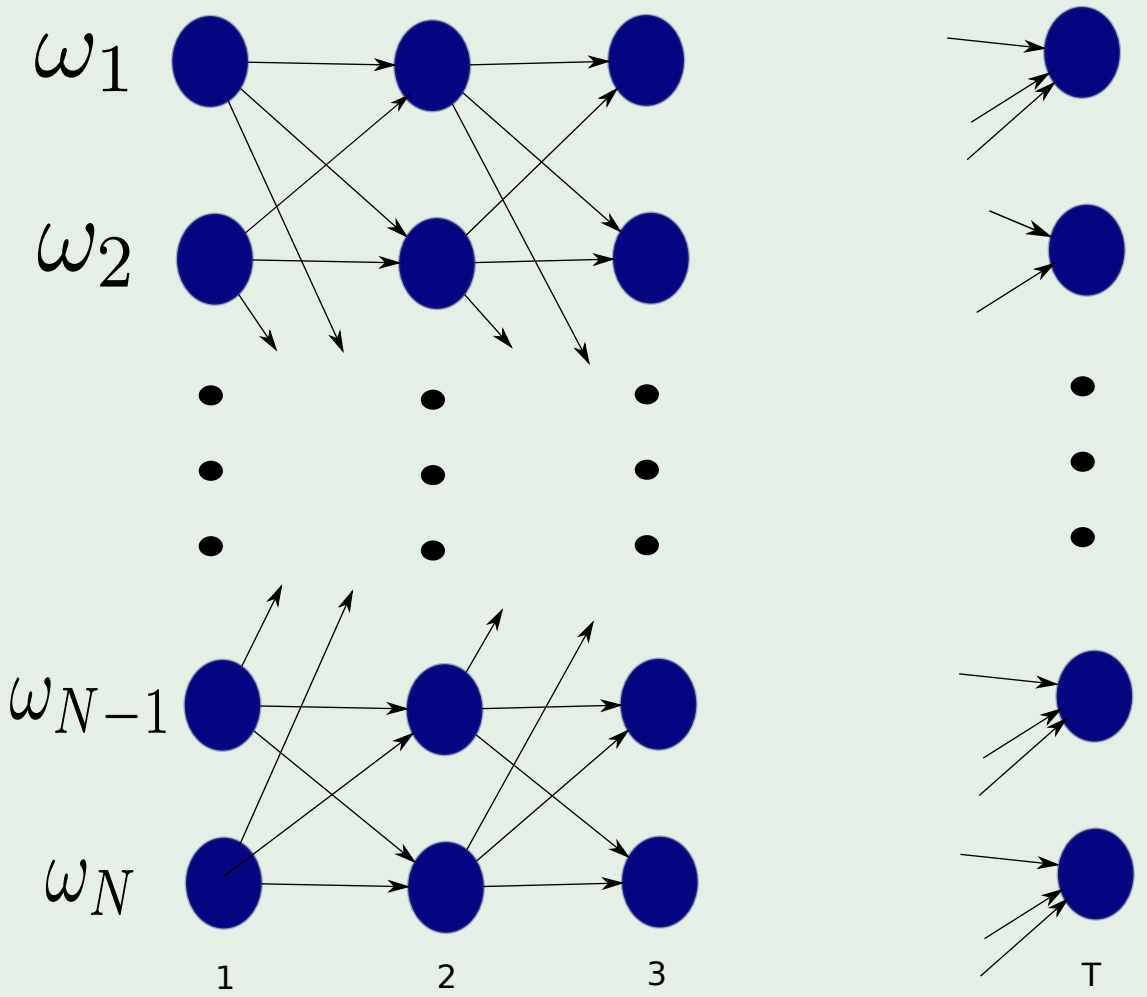
We have

1. Inner loop $O(N)$
2. Outer loop $O(NT)$
   - Then $O(N^2T)$

Outline

All this come from the Lattice Structure

Lattice with Lenght T over time and Depth N over the structure of the probabilistic state machine



Notice the following

The forward method

It is enough to solve the first problem.

However for the second problem

We need to define the backward variable,

$$\beta_t(i) = P(x_{t+1}, x_{t+2}, \ldots, x_T | q_t = \omega_i, \lambda).$$

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This can be solved in a similar way

Initialization

$$\beta_T(i) = 1, \ 1 \leq i \leq N \tag{24}$$

Induction

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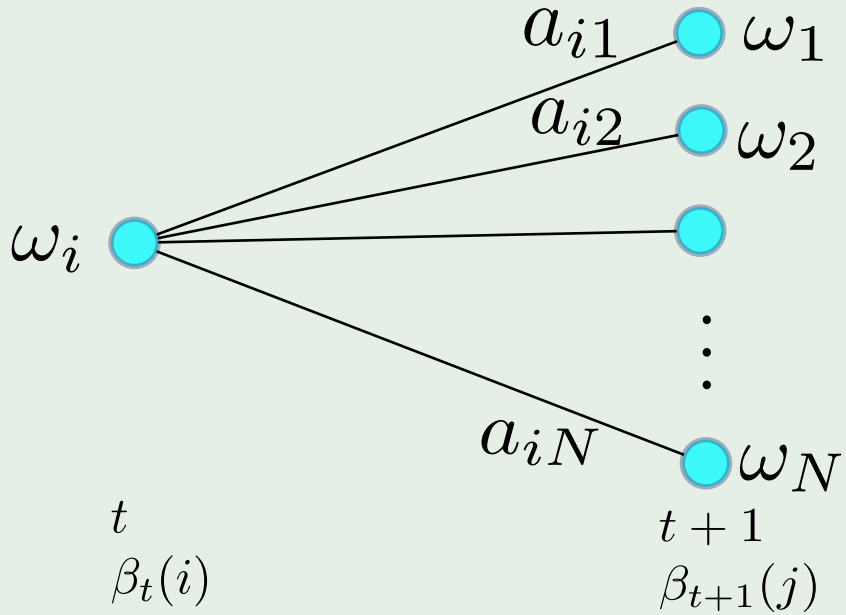
Example of the backward process

Example



How?

That is for the next midterm

Please try it for yourselves!!!

Outline

Here, we have several ways of solving the problem

Problem

Given the observation sequence X and a model λ, How we choose a corresponding class sequence Ω?

For this, we define

$$\gamma_t(i) = P(q_t = \omega_i | X, \lambda) \tag{26}$$

Meaning

The probability of being in state ω_i at time t given the observation sequence X and the model λ.

Here, we have several ways of solving the problem

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Meaning

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We can find its meaning using Bayes

We get

$$\gamma_t(i) = \frac{P(x_1, ..., x_t, ..., x_T, q_t = \omega_i|\lambda)}{P(x_1, ..., x_t, ..., x_T|\lambda)}$$

$$= \frac{P(x_1, ..., x_t, q_t = \omega_i, x_{t+1} ..., x_T|\lambda)}{P(x_1, ..., x_t, ..., x_T|\lambda)}$$

$$= \frac{P(x_1, ..., x_t, x_{t+1} ..., x_T|q_t = \omega_i, \lambda) P(q_t = \omega_i|\lambda)}{P(x_1, ..., x_t, ..., x_T|\lambda)}$$

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We can find its meaning using Bayes

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In addition, we have that

The $\gamma_t(i)$ are a probability because

$$\sum_{i=1}^{N} \gamma_t(i) = 1 \tag{27}$$

Thus, we can use this to generate the most likely state q_t at time t

$$q_t = \text{argmax}_{1 \leq i \leq N} [\gamma_t(i)], \text{ for } 1 \leq t \leq T \tag{28}$$

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Outline

What can we use? Dynamic Programming

Optimal Substructure

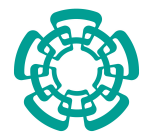
Optimal solution to sub-problems.

Overlapping Sub-problems

Use previous solutions to reduce complexity.

Finally

Reconstructing an optimal solution.



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Optimal Substructure Process

Process

- Show that a solution to the problem consists of making a choice. It leaves a sub-problem to solve.
- Given a problem you suppose an optimal solution.
- Given this choice you determine how to solve the sub-problems.
- Then, you determine that the solution to the sub-problem is optimal by contradiction.

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Possible Solutions

One Optimal Criteria

It is possible to to solve for the state sequences that maximizes the expected number of correct pairs of states (q_t, q_{t+1})

However

The most widely criteria is to find the single best path to maximize $P(\Omega|X,\lambda) \approx P(\Omega,X|\lambda)$

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Outline

Viterbi Algorithm

Setup

We want the best single state sequence $\Omega_i = \{\omega_{i_1}, \omega_{i_2}, ..., \omega_{i_T}\}$ for a given observation X

Thus, we define

$$\delta_t(i) = \max_{q_1, q_2, ..., q_{t-1}} P[q_1, q_2, \cdots, q_t = i, x_1, x_2, \cdots, x_t | \lambda] \quad (29)$$

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Use Induction

We can do the following

$$\delta_{t+1}(j) = \max_{q_1, q_2, \ldots, q_t} P[q_1, q_2, \cdots, q_{t+1} = j, x_1, x_2, \cdots, x_{t+1} | \lambda]$$

$$= \max_i \{P[q_{t+1} = j, x_{t+1} | q_1, q_2, \cdots, q_t = i, x_1, x_2, \cdots, x_t, \lambda] \times \cdots$$

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Procedure

Initialization

- $\delta_1(i) = \pi_i b_i(x_1),\ 1 \leq i \leq N$
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- $\delta_1(i) = \pi_i b_i(x_1)$, $1 \leq i \leq N$
- Array $\Psi_1(i) = 0$, $1 \leq i \leq N$

Recusrions

- $\delta_t(j) = \max_{1 \leq i \leq N} \left[a_{ij} \delta_{t-1}(i) \right] b_j(x_t)$, $2 \leq t \leq T$ and $1 \leq j \leq N$
- $\Psi_t(j) = \text{argmax}_{1 \leq i \leq N} \left[a_{ij} \delta_{t-1}(i) \right]$, $2 \leq t \leq T$ and $1 \leq j \leq N$

Termination

- $P* = \max_{1 \leq i \leq N} \left[\delta_T(i) \right]$
- $q_T* = \text{argmax}_{1 \leq i \leq N} \left[\delta_T(i) \right]$

Clearly

Something Notable

All those recursion can be changed for iterative bottom-up procedure

That all

I leave to you to figure out!!!

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Backtracking

Path backtracking

$q_t* = \Psi_{t+1}(q_{t+1}*)$, $t = T-1, T-2, \cdots, 1$.

Outline

The most difficult

Problem

There is no analytical solution to third problem!!!

However

Given a finite observation sequence as trainign data, we can choose $\lambda(A, B, \pi)$ such that $P(O|\lambda)$is maximized.

For this

We have the Baum-Welch or Forward-Backward Algorithm.

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Another way to see this is thinking in Maximum Likelihood

Given our observed data sequence $X = \langle x_1, x_2, ..., x_T \rangle$

The likelihood function is obtained from the joint distribution by marginalizing over the Hidden State Variables

$$P(X|\lambda) = \sum_{\Omega} P(X, \Omega|\lambda) \tag{30}$$

Problems

- We cannot simply treat each summation over ω_i independently!!!
- We cannot perform all the summations explicitly because it results in N^T terms.

And Again

A further difficulty for the likelihood function is that represents a summation over the emission models for different settings of the latent variables.

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Initial Setup

Let us consider discrete (categorical) HMMs of length T (each observation sequence is T observations long).

1. N is the number of hidden states.
2. M is the number of different observation symbols.
3. D observations, $\mathcal{X} = \left\{X^{(1)}, X^{(2)}, ..., X^{(D)}\right\}$ such that $X^{(i)} = \left\{x_1^{(i)}, x_2^{(i)}, ..., x_T^{(i)}\right\}$.
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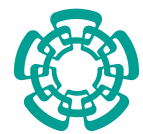

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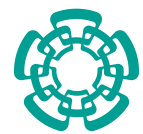

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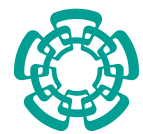

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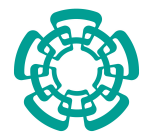

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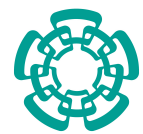

Outline

Baum-Welch Algorithm

Remember the EM Algorithm

1. Compute $Q(\lambda, \lambda^n) = \sum_{\mathbf{\Omega}} \log [P(\mathcal{X}, \mathbf{\Omega}|\lambda)] P(\mathbf{\Omega}|\mathcal{X}, \lambda^n)$
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Cinvestav

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We know that

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Now, assuming we have D observations

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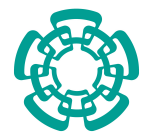
Thus

We have

$$P\left(\mathcal{X}, \mathbf{\Omega}|\lambda\right) = \prod_{d=1}^{D}\left[\prod_{t=1}^{T} P\left(x_t^{(d)}|\omega_t^{(d)}, \lambda\right)\left[\prod_{t=2}^{T} P\left(\omega_t^{(d)}|\omega_{t-1}^{(d)}, \lambda\right)\right] P\left(\omega_1^{(d)}|\lambda\right)\right]$$

$$= \prod_{d=1}^{D}\left[\pi_{q_1^{(d)}} b_{q_1^{(d)}}\left(x_1^{(d)}\right)\left[\prod_{t=2}^{T} a_{q_{t-1}^{(d)} q_t^{(d)}} b_{q_t^{(d)}}\left(x_t^{(d)}\right)\right]\right]$$



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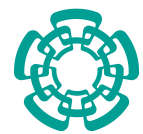

Now, taking the logarithm

We get

$$\log P(\mathcal{X}, \mathbf{\Omega}|\lambda) = \sum_{d=1}^{D} \left[\log \pi_{q_1^{(d)}} + \ldots \right.$$
$$\sum_{t=2}^{T} \log a_{q_{t-1}^{(d)} q_t^{(d)}} + \ldots$$
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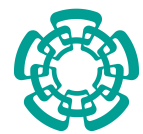
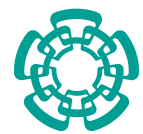


We plug back into $\hat{Q}(\lambda, \lambda^n)$

We get the following

$$\begin{aligned}\hat{Q}(\lambda, \lambda^n) = &\sum_{\mathbf{\Omega}} \sum_{d=1}^{D} \log \pi_{q_1^{(d)}} P(\mathbf{\Omega}, \mathcal{X}|\lambda^n) \\ &\sum_{\mathbf{\Omega}} \sum_{d=1}^{D} \sum_{t=2}^{T} \log a_{q_{t-1}^{(d)} q_t^{(d)}} P(\mathbf{\Omega}, \mathcal{X}|\lambda^n) + ... \\ &\sum_{\mathbf{\Omega}} \sum_{d=1}^{D} \sum_{t=1}^{T} \log b_{q_t^{(d)}}\left(x_t^{(d)}\right) P(\mathbf{\Omega}, \mathcal{X}|\lambda^n)\end{aligned}$$



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- It looks like it will increase the complexity of our calculations

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Using marginalization, we will be able to remove the terms that are not necessary to calculate the necessary updates.

Which Updates?

π_i , a_{ij} and $b_j(k)$

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Now, Which Lagrange Multipliers?

One for the M hidden marginal states of π

$$\sum_{i=1}^{N} \pi_i = 1 \tag{31}$$

One for each i

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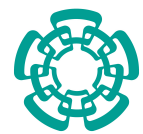
Finally, we have the new Lagrangian

We have

$$\hat{L}\left(\lambda,\lambda^{n}\right)=\hat{Q}\left(\lambda,\lambda^{n}\right)-\lambda_{\pi}\left(\sum_{i=1}^{N}\pi_{i}-1\right)-\sum_{i=1}^{N}\lambda_{a_{i}}\left(\sum_{j=1}^{N}a_{ij}-1\right)-\sum_{i=1}^{N}\lambda_{b_{i}}\left(\sum_{k=1}^{M}b_{i}\left(k\right)-1\right)$$

Outline



Now, if we derive with respect to π_i

We have that

$$\frac{\partial \hat{L}(\lambda, \lambda^n)}{\partial \pi_i} = \frac{\partial}{\partial \pi_i}\left(\sum_{\mathbf{\Omega}}\sum_{d=1}^{D} \log \pi_{q_1^{(d)}} P(\mathbf{\Omega}, \mathcal{X}|\lambda^n)\right) - \lambda_\pi$$

$$= \frac{\partial}{\partial \pi_i}\left(\sum_{j=1}^{N}\sum_{d=1}^{D} \log \pi_j P\left(q_1^{(d)} = j, \mathcal{X}|\lambda^n\right)\right) - \lambda_\pi$$

$$= \frac{1}{\pi_i}\sum_{d=1}^{D} P\left(q_1^{(d)} = i, \mathcal{X}|\lambda^n\right) - \lambda_\pi = 0$$

Remark: The second step is simply the result of marginalizing out, for each d, all $q_{t\neq 1}^{(d)}$ and $q_t^{(d'\neq d)}$ for all t.

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Remark: The second step is simply the result of marginalizing out, for each d, all $q_{t\neq 1}^{(d)}$ and $q_t^{(d'\neq d)}$ for all t.

Now, if we derive with respect to π_i

We have that

$$\begin{aligned}\frac{\partial \hat{L}(\lambda, \lambda^n)}{\partial \pi_i} &= \frac{\partial}{\partial \pi_i}\left(\sum_{\mathbf{\Omega}}\sum_{d=1}^{D} \log \pi_{q_1^{(d)}} P(\mathbf{\Omega}, \mathcal{X}|\lambda^n)\right) - \lambda_\pi \\ &= \frac{\partial}{\partial \pi_i}\left(\sum_{j=1}^{N}\sum_{d=1}^{D} \log \pi_j P\left(q_1^{(d)} = j, \mathcal{X}|\lambda^n\right)\right) - \lambda_\pi \\ &= \frac{1}{\pi_i}\sum_{d=1}^{D} P\left(q_1^{(d)} = i, \mathcal{X}|\lambda^n\right) - \lambda_\pi = 0\end{aligned}$$

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After all

$$\sum_{d=1}^{D} \log \pi_{q_1^{(d)}} \sum_{\Omega} P\left(\mathbf{\Omega}, \mathcal{X}|\lambda^n\right) = \sum_{d=1}^{D} \log \pi_{q_1^{(d)}} \sum_{j_1^1=1}^{N} \sum_{j_2^1=1}^{N} \cdots \sum_{j_T^1=1}^{N} \cdots \sum_{j_1^T=1}^{N} \sum_{j_2^T=1}^{N} \cdots \sum_{j_T^T=1}^{N} P\left(\mathbf{\Omega}, \mathcal{X}|\lambda^n\right)$$

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Thus we have

$$\pi_i = \frac{1}{\lambda_\pi} \sum_{d=1}^{D} P\left(q_1^{(d)} = i, \mathcal{X}|\lambda^n\right) \tag{34}$$

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Now deriving against λ_π

We have that

$$\sum_{i=1}^{N} \pi_i = 1 \tag{35}$$

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$$\frac{1}{\lambda_\pi} \sum_{i=1}^{N} \sum_{d=1}^{D} P\left(q_1^{(d)} = i, \mathcal{X} | \lambda^n\right) = 1 \tag{36}$$

Then

$$\lambda_\pi = \sum_{i=1}^{N} \sum_{d=1}^{D} P\left(q_1^{(d)} = i, \mathcal{X} | \lambda^n\right) \tag{37}$$

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Plugging back

We get

$$\frac{1}{\pi_i}\sum_{d=1}^{D} P\left(q_1^{(d)}=i,\mathcal{X}|\lambda^n\right)-\lambda_\pi=0$$

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In addition

We can modify our γ

$$\gamma_{q_{t-1}^{(d)}}(i) = P\left(q_{t-1}^{(d)} = i | X^{(d)}, \lambda^n\right) \tag{38}$$

Meaning

The probability of being in state i at time $q_{t-1}^{(d)}$ given the observation sequence $X^{(d)}$ and the model λ^n.

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Meaning

The probability of being in state i at time $q_{t-1}^{(d)}$ given the observation sequence $X^{(d)}$ and the model λ^n.

Thus

We have

$$\pi_i = \frac{\sum_{d=1}^{D} P\left(\mathcal{X}|\lambda^n\right) P\left(q_1^{(d)} = i|\mathcal{X}, \lambda^n\right)}{DP\left(\mathcal{X}|\lambda^n\right)}$$

$$\pi_i = \frac{1}{D}\sum_{d=1}^{D} P\left(q_1^{(d)} = i|X^{(d)}, \lambda^n\right)$$

$$\pi_i = \frac{1}{D}\sum_{d=1}^{D} \gamma_{q_1^{(d)}}(i)$$

Remark: This can be thought as the expected frequency (Number of Times) in state i at time $(t = 1) = \gamma_{q_1^{(d)}}(i)$

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Now, for a_{ij}

We now follow a similar process for the a_{ij}

$$\frac{\partial \hat{L}(\lambda, \lambda^n)}{\partial a_{ij}} = \frac{\partial}{\partial a_{ij}} \left(\sum_{\mathbf{\Omega}} \sum_{d=1}^{D} \sum_{t=2}^{T} \log a_{q_{t-1}^{(d)} q_t^{(d)}} P(\mathbf{\Omega}, \mathcal{X} | \lambda^n) \right) - \sum_{i=1}^{N} \lambda_{a_i}$$

$$= \frac{\partial}{\partial a_{ij}} \left(\sum_{h=1}^{N} \sum_{k=1}^{N} \sum_{d=1}^{D} \sum_{t=2}^{T} \log a_{jk} P\left(q_{t-1}^{(d)} = h, q_t^{(d)} = k, \mathcal{X} | \lambda^n\right) \right) - \lambda_{a_i}$$

$$= \frac{1}{a_{ij}} \sum_{d=1}^{D} \sum_{t=2}^{T} P\left(q_{t-1}^{(d)} = i, q_t^{(d)} = j, \mathcal{X} | \lambda^n\right) - \lambda_{a_i} = 0$$

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Then

We have that

$$a_{ij} = \frac{\sum_{d=1}^{D}\sum_{t=2}^{T} P\left(q_{t-1}^{(d)} = i, q_t^{(d)} = j, \mathcal{X}|\lambda^n\right)}{\lambda_{a_i}}$$

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Then, using $\sum_{j=1}^{N} a_{ij} = 1$

$$\lambda_{a_i} = \sum_{j=1}^{N}\sum_{d=1}^{D}\sum_{t=2}^{T} P\left(q_{t-1}^{(d)} = i, q_t^{(d)} = j, \mathcal{X}|\lambda^n\right) \tag{40}$$

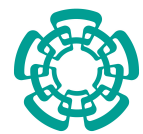
Re-expressing

We get

$$a_{ij} = \frac{\sum_{d=1}^{D}\sum_{t=2}^{T} P\left(q_{t-1}^{(d)} = i, q_{t}^{(d)} = j, \mathcal{X}|\lambda^n\right)}{\sum_{j=1}^{N}\sum_{d=1}^{D}\sum_{t=2}^{T} P\left(q_{t-1}^{(d)} = i, q_{t}^{(d)} = j, \mathcal{X}|\lambda^n\right)}$$

Marginalizing the denominator and numerator in $\mathcal{X}$

$$a_{ij} = \frac{\sum_{d=1}^{D}\sum_{t=2}^{T} P\left(q_{t-1}^{(d)} = i, q_{t}^{(d)} = j, \mathcal{X}|\lambda^n\right)}{\sum_{d=1}^{D}\sum_{t=2}^{T} P\left(q_{t-1}^{(d)} = i, \mathcal{X}|\lambda^n\right)}$$



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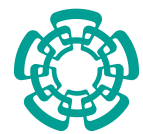
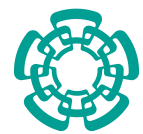


Next

We have

$$a_{ij} = \frac{\sum_{d=1}^{D}\sum_{t=2}^{T} P\left(q_{t-1}^{(d)} = i, q_t^{(d)} = j|\mathcal{X}, \lambda^n\right) P\left(\mathcal{X}|\lambda^n\right)}{\sum_{d=1}^{D}\sum_{t=2}^{T} P\left(q_{t-1}^{(d)} = i|\mathcal{X}, \lambda^n\right) P\left(\mathcal{X}|\lambda^n\right)}$$

$$= \frac{\sum_{d=1}^{D}\sum_{t=2}^{T} P\left(q_{t-1}^{(d)} = i, q_t^{(d)} = j|X^{(d)}, \lambda^n\right)}{\sum_{d=1}^{D}\sum_{t=2}^{T} P\left(q_{t-1}^{(d)} = i|X^{(d)}, \lambda^n\right)}$$



Now, we are looking for a more compact version

We define

The probability of being in state i at time $q_{t-1}^{(d)}$ and state j at time $q_t^{(d)}$:

$$\xi_{q_{t-1}^{(d)}}(i,j) = P\left(q_{t-1}^{(d)} = i, q_t^{(d)} = j | X^{(d)}, \lambda\right) \tag{41}$$

This is Basically a Joint Probability

We have

- A Joint Probability over $q_{t-1}^{(d)} = i$ and $q_t^{(d)} = j$ given data sample $X^{(d)}$

A question raises immediately

- To what is this equivalent?

For this

- We can use Bayes!!!

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Using Bayes

We have for $\xi_{q_{t-1}^{(d)}}(i,j)$

$$\xi_{q_{t-1}^{(d)}}(i,j) = \frac{P\left(x_1^{(d)},\ldots,x_{t-1}^{(d)},q_{t-1}^{(d)}=i,q_t^{(d)}=j,x_t^{(d)},\ldots,x_T^{(d)}|X^{(d)},\lambda\right)}{P\left(X^{(d)}|\lambda\right)}$$

$$= \frac{P\left(x_1^{(d)},\ldots,x_{t-1}^{(d)},q_{t-1}^{(d)}=i|q_t^{(d)}=j,x_t^{(d)},\ldots,x_T^{(d)},\lambda\right)P\left(q_t^{(d)}=j,x_t^{(d)},\ldots,x_T^{(d)}|\lambda\right)}{P\left(X|\lambda\right)}$$

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$$\frac{P\left(q_t^{(d)}=j,x_t^{(d)}|\lambda\right)}{}$$

$$= P\left(x_1^{(d)},\cdots,x_{t-1}^{(d)},q_{t-1}^{(d)}=i|q_t^{(d)}=j,\lambda\right)P\left(x_{t+1}^{(d)},\cdots,x_T^{(d)}|q_t^{(d)}=j,x_t^{(d)},\lambda\right)\times\cdots$$

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Using Bayes

We have for $\xi_{q_{t-1}^{(d)}}(i,j)$

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Again Bayes

Thus $\xi_{q_{t-1}^{(d)}}(i,j) =$

$$= \frac{P\left(x_1^{(d)}, ..., x_{t-1}^{(d)}, q_{t-1}^{(d)} = i, q_t^{(d)} = j|\lambda\right) \beta_t(j) b_j(x_t)}{P\left(X^{(d)}|\lambda\right)}$$

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$$= \frac{P\left(q_t^{(d)} = j|q_{t-1}^{(d)} = i, \lambda\right) \alpha_{t-1}^{(d)}(i) \beta_t^{(d)}(j) b_j\left(x_t^{(d)}\right)}{P\left(X^{(d)}|\lambda\right)}$$

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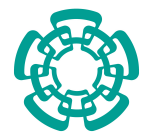

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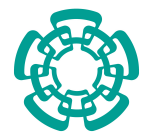

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Basically an Aggregation

Of the probabilities

- One coming from the Past of sample $X^{(d)}$

$$\text{Information from the Past} = \alpha_{t-1}^{(d)}(i)$$

Ones coming from the Future of sample $X^{(d)}$

$$\text{Information from the Future} = \beta_t^{(d)}(j)$$

Basically an Aggregation

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$$\text{Information from the Past} = \alpha_{t-1}^{(d)}(i)$$

Ones coming from the Future of sample $X^{(d)}$

$$\text{Information from the Future} = \beta_{t}^{(d)}(j)$$

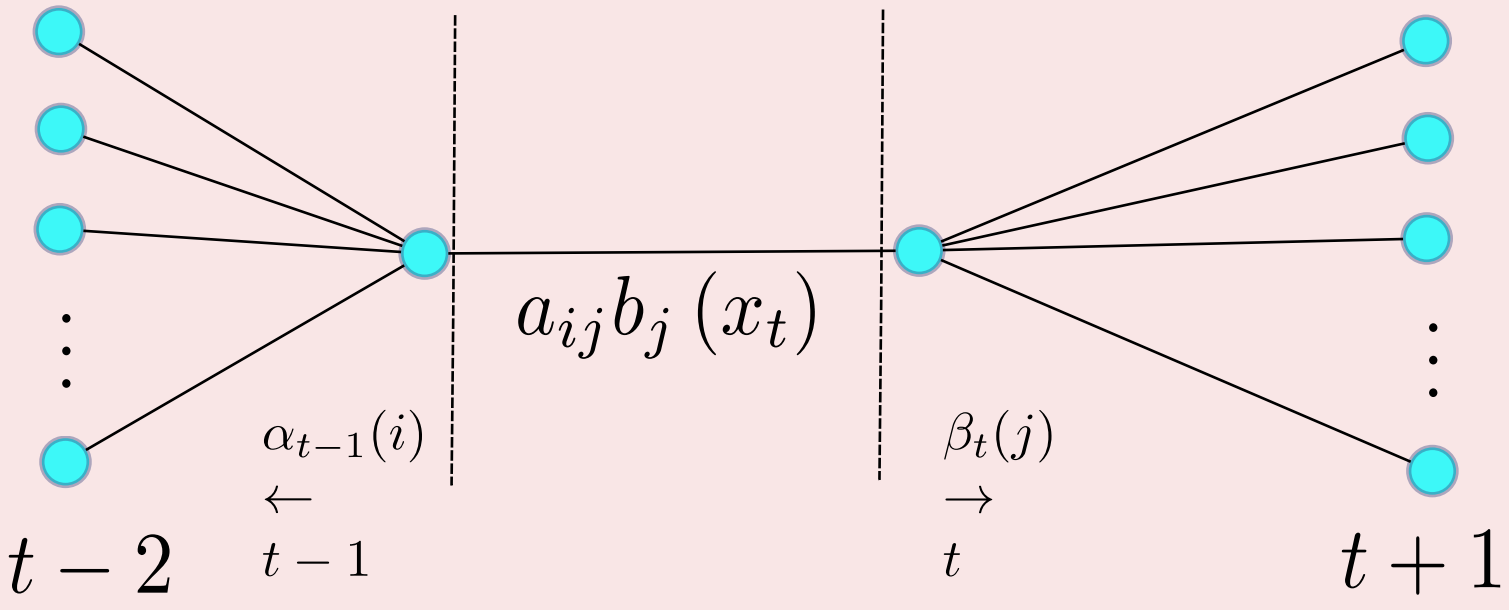
Thus

To reach the symbol $x_t^{(d)}$ at sample $X^{(d)}$

Information when reaching state i and emiting $x_t = a_{ij}^{(d)} b_j \left(x_t^{(d)} \right)$

This can be seen graphically as

This is illustrated by the following figure



In addition

Given the definition of $\gamma_{q_{t-1}^{(d)}}(i)$

$$\gamma_{q_{t-1}^{(d)}}(i) = \frac{\alpha_{q_{t-1}^{(d)}}(i)\,\beta_{q_{t-1}^{(d)}}(i)}{\sum_{j=1}^{N}\alpha_{q_t^{(d)}}(j)\,\beta_{q_t^{(d)}}(j)} \tag{42}$$

Summing over j

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Summing over j

$$\sum_{j=1}^{N}\xi_{q_{t-1}^{(d)}}(i,j) = \sum_{j=1}^{N}P\left(q_{t-1}^{(d)} = i, q_t^{(d)} = j | X^{(d)}, \lambda\right)$$

$$= P\left(q_{t-1}^{(d)} = i | X^{(d)}, \lambda\right)$$

$$= \frac{P\left(x_1^{(d)}, \cdots, x_{t-1}^{(d)}, q_{t-1}^{(d)} = i, x_t^{(d)}, \cdots, x_T^{(d)} | \lambda\right)}{P\left(X^{(d)} | \lambda\right)}$$

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Summing over j

$$\begin{aligned}\sum_{j=1}^{N}\xi_{q_{t-1}^{(d)}}(i,j) &= \sum_{j=1}^{N} P\left(q_{t-1}^{(d)} = i, q_t^{(d)} = j | X^{(d)}, \lambda\right) \\ &= P\left(q_{t-1}^{(d)} = i | X^{(d)}, \lambda\right)\end{aligned}$$

$$= \frac{P\left(x_1^{(d)}, \cdots, x_{t-1}^{(d)}, q_{t-1}^{(d)} = i, x_t^{(d)}, \cdots, x_T^{(d)} | \lambda\right)}{P\left(X^{(d)} | \lambda\right)}$$

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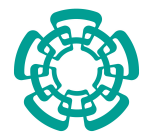
Then

We have

$$= \frac{P\left(x_1^{(d)}, ..., x_{t-1}^{(d)}, q_{t-1}^{(d)} = i, x_t^{(d)}, ..., x_T^{(d)} | \lambda\right)}{P\left(X^{(d)} | \lambda\right)}$$

$$= \frac{\alpha_{t-1}(i)\,\beta_{t-1}(i)}{\sum_{i=1}^{N} P\left(x_1, ..., x_t, ..., x_T, q_t = \omega_i | \lambda\right)}$$

$$= \gamma_{q_{t-1}^{(d)}}(i)$$



Then

We have

$$
\begin{aligned}
&= \frac{P\left(x_1^{(d)}, ..., x_{t-1}^{(d)}, q_{t-1}^{(d)} = i, x_t^{(d)}, ..., x_T^{(d)} | \lambda\right)}{P\left(X^{(d)} | \lambda\right)} \\
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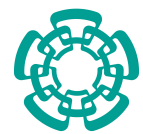

We can also think about the expected values

The following sum

1. It can be thought as expected (over time) number of times that state ω_i is visited
2. Or the number of transitions made from state ω_i

It is

$$\sum_{t=2}^{T} \gamma_{q_{t-1}^{(d)}}(i) \tag{43}$$

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Also the expected value for $\xi_{q_{t-1}^{(d)}}(i,j)$

The following sum

It can be thought as the expected number of transitions from i to j

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$$\sum_{t=2}^{T} \xi_{q_{t-1}^{(d)}}(i,j) \tag{44}$$

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The following sum

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$$\sum_{t=2}^{T} \xi_{q_{t-1}^{(d)}}(i,j) \tag{44}$$

Remark

Important

Baum et al. proved that the maximization of$Q\left(\lambda,\overline{\lambda}\right)$ leads to increased likelihood:

$$\max_{\overline{\lambda}}\left[Q\left(\lambda,\overline{\lambda}\right)\right]\Rightarrow P\left(X|\overline{\lambda}\right)\geq P\left(X|\lambda\right) \tag{45}$$

For details

Please look back at our slides on EM!!!

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We can rewrite a_{ij}

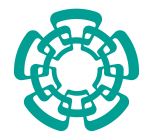
Thus

$$a_{ij} = \frac{\sum_{d=1}^{D}\sum_{t=2}^{T} P\left(q_{t-1}^{(d)} = i, q_{t}^{(d)} = j | X^{(d)}, \lambda^{n}\right)}{\sum_{d=1}^{D}\sum_{t=2}^{T} P\left(q_{t-1}^{(d)} = i | X^{(d)}, \lambda^{n}\right)}$$

$$= \frac{\sum_{d=1}^{D}\sum_{t=2}^{T} \xi_{q_{t-1}^{(d)}}(i,j)}{\sum_{d=1}^{D}\sum_{t=2}^{T} \gamma_{q_{t-1}^{(d)}}(i)}$$

Remark: This can be seen as

- $\frac{\text{expected number of transitions from state } i \text{ to } j}{\text{expected number of transitions made from state } i}$



Now, the terms $b_i(k)$

We have that

$$\frac{\partial \hat{L}(\lambda, \lambda^n)}{\partial b_i(k)} = \frac{\partial}{\partial b_i(k)} \left(\sum_{\mathbf{\Omega}} \sum_{d=1}^{D} \sum_{t=1}^{T} \log b_{q_t^{(d)}} \left(x_t^{(d)} \right) P(\mathbf{\Omega}, \mathcal{X} | \lambda^n) \right) - \lambda_{b_i}$$

$$= \frac{\partial}{\partial b_i(k)} i, \left(\sum_{h=1}^{N} \sum_{d=1}^{D} \sum_{t=1}^{T} \log b_h \left(x_t^{(d)} \right) P\left(q_t^{(d)} = h, \mathcal{X} | \lambda^n \right) \right) - \lambda_{b_i}$$

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Now, we have a problem

The term $b_i(k)$ can be different than term $b_i\left(x_t^{(d)}\right)$

We can use this to fix our problem

$$I\left(x_t^{(d)} = k\right) = \begin{cases} 1 & \text{when } x_t^{(d)} == k \\ 0 & \text{Otherwise} \end{cases} \tag{46}$$

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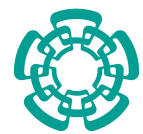
Thus, we have that

Using our previous idea

$$\frac{\partial \hat{L}(\lambda, \lambda^n)}{\partial b_i(k)} = \sum_{d=1}^{D}\sum_{t=1}^{T} \frac{P\left(q_t^{(d)} = i, \mathcal{X}|\lambda^n\right) I\left(x_t^{(d)} = k\right)}{b_i(k)} - \lambda_{b_i}$$

In addition

$$\frac{\partial \hat{L}(\lambda, \lambda^n)}{\partial \lambda_{b_i}} = -\left(\sum_{k=1}^{M} b_i(k) - 1\right) \tag{47}$$



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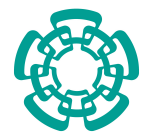

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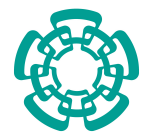

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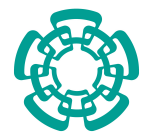

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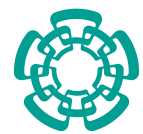

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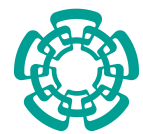

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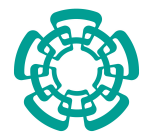

Using Rabiner's Notation

We have that

$$b_i(k) = \frac{\sum_{d=1}^{D}\sum_{t=1}^{T}\gamma_{q_t^{(d)}}(i)\, I\left(x_t^{(d)} = k\right)}{\sum_{d=1}^{D}\sum_{t=1}^{T}\gamma_{q_t^{(d)}}(i)} \tag{50}$$

Which can be seen as

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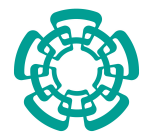
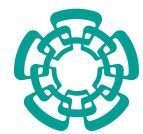


Outline



Thus, the re-estimation

First

$$\pi_i^{(n+1)} = \frac{1}{D}\sum_{d=1}^{D}\gamma_{q_1^{(d)}}(i) \tag{51}$$

Second

$$a_{ij}^{(n+1)} = \frac{\sum_{d=1}^{D}\sum_{t=2}^{T}\xi_{q_{t-1}^{(d)}}(i,j)}{\sum_{d=1}^{D}\sum_{t=2}^{T}\gamma_{q_{t-1}^{(d)}}(i)} \tag{52}$$

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Something Nice

An important aspect of the re-estimation procedure is that

$$\sum_{i=1}^{N} \pi_i^{(n+1)} = 1$$

$$\sum_{j=1}^{N} a_{ij}^{(n+1)} = 1 \; 1 \leq i \leq N$$

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Automatically it is satisfied at each iteration.

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Outline

Once these probabilities are ready

We can use Naïve Bayes

$$P(\Omega_i|X) = \frac{P(\Omega_i, X)}{P(X)} > \frac{P(\Omega_j, X)}{P(X)} = P(\Omega_j|X) \ \forall i \neq j \tag{54}$$

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