Markov Chain,Hidden Markov Model

March 21, 2016

Discrete-time Markov chains

- Definition: A Markov chain is a discrete-time stochastic process $(X_n, n \geq 0)$ such that each random variable X_n takes values in a discrete set S ($S = N$, typically) and

$$P(X_{n+1} = j | X_n = i, X_{n-1} = i_{n-1}, \cdots, X_0 = i_0) = P(X_{n+1} = j | X_n = i),$$

$$\forall n \geq 0, j, i, i_{n-1}, \cdots, i_0 \in S$$

- If $P(X_{n+1} = j | X_n = i) = p_{ij}$ is independent of n, then X is said to be a time-homogeneous Markov chain.

- Terminology
  The possible values taken by the random variables X_n are called the states of the chain. S is called the state space.
  The chain is said to be finite-state if the set S is finite ($S = \{0, \cdots, N\}$, typically).
  $P = (p_{ij})\ i, j \in S$ is called the transition matrix of the chain.
- Properties of the transition matrix

$$p_{ij} \geq 0, \forall i, j \in S$$

$$\sum_{\forall j \in S} p_{ij} = 1, \forall i \in S.$$

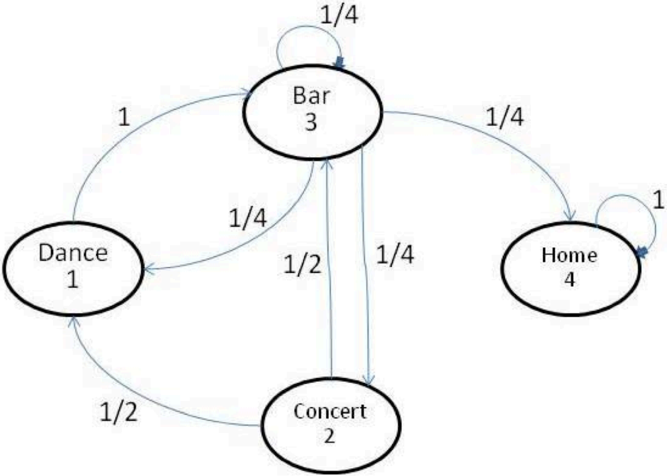
Example 1: Music Festival

- The four possible states of a student in a music festival are S = "dancing", "at a concert", "at the bar", "back home". Let us assume that the student changes state during the festival according to the following transition matrix:

$$P = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 1/2 & 0 & 1/2 & 0 \\ 1/4 & 1/4 & 1/4 & 1/4 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

Example

The Markov chain can be represented by the following transition graph:



Example 2: Simple symmetric random walk

- Let $(X_n, n \geq 1)$ be i.i.d. random variables such that $P(X_n = +1) = P(X_n = -1) = 1/2$, and let $(S_n, n \geq 0)$ be defined as $S_0 = 0, S_n = X_1 + \cdots + X_n, n \geq 1$. Then $(S_n, n \in N)$ is a Markov chain with state space $S = Z$.

- Indeed:

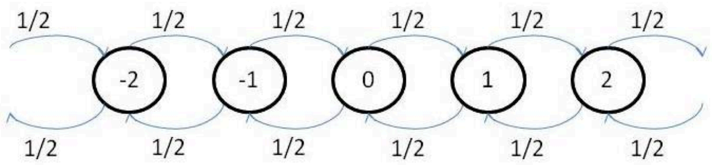
$$P(S_{n+1} = j | S_n = i, S_{n-1} = i_{n-1}, \cdots, S_0 = i_0)$$

$$= P(X_{n+1} = j - i | S_n = i, S_{n-1} = i_{n-1}, \cdots, S_0 = i_0) = P(X_{n+1} = j - i)$$

by the assumption that the variables X_n are independent.

- The chain is time-homogeneous, as $P(X_{n+1} = j - i) = 1/2$, if $|j - i| = 1$,$P(X_{n+1} = j - i) = 0$, otherwise, which does not depend on n.

The transition graph of the chain:



- The distribution at time *n* of the Markov chain *X* is given by:

$$\pi_i^{(n)} = P(X_n = i), i \in S.$$

- We know that $\pi_i^{(n)} \geq 0 \ \forall i \in S$ and that $\sum_{i \in S} \pi_i^{(n)} = 1$.
- The initial distribution of the chain is given by $\pi_i^{(0)} = P(X_0 = i), i \in S$.
- It must be specified together with the transition matrix $P = (p_{ij}), i, j \in S$ in order to characterize the chain completely.

$$
\begin{aligned}
& P(X_n = i_n, X_{n-1} = i_{n-1}, \cdots, X_1 = i_1, X_0 = i_0) \\
= \; & P(X_n = i_n | X_{n-1} = i_{n-1}, \cdots, X_1 = i_1, X_0 = i_0) \cdot \\
& P(X_{n-1} = i_{n-1}, \cdots, X_1 = i_1, X_0 = i_0) \\
= \; & p_{i_{n-1}, i_n} P(X_{n-1} = i_{n-1}, \cdots, X_1 = i_1, X_0 = i_0) \\
= \; & \cdots = p_{i_{n-1}, i_n} p_{i_{n-2}, i_{n-1}} \cdots p_{i_1, i_2} p_{i_0, i_1} \pi(0)
\end{aligned}
$$

So knowing P and knowing $\pi(0)$ allows to compute all the above probabilities, which give a complete description of the process.

The n-step transition probabilities of the chain are given by

$$p_{ij}^{(n)} = P(X_{m+n} = j | X_m = i), n, m \geq 0, i, j \in S.$$

Let us compute:

$$\begin{aligned}
p_{ij}^{(2)} &= P(X_{n+2} = j | X_n = i) = \sum_{k \in S} P(X_{n+2} = j, X_{n+1} = k | X_n = i) \\
&= \sum_{k \in S} P(X_{n+2} = j | X_{n+1} = k, X_n = i) \cdot P(X_{n+1} = k | X_n = i) \\
&= \sum_{k \in S} P(X_{n+2} = j | X_{n+1} = k) \cdot P(X_{n+1} = k | X_n = i) \\
&= \sum_{k \in S} p_{ik} p_{kj}
\end{aligned}$$

The Chapman-Kolmogorov equation for generic values of m and n:

$$p_{ij}^{(n+m)} = \sum_{k \in S} p_{ik}^{(n)} p_{kj}^{(m)}, i, j \in S, n, m \geq 0,$$

where we define by convention $p_{ij}^{(0)} = \delta_{ij} = 1$, if $i = j$, $p_{ij}^{(0)} = \delta_{ij} = 0$ otherwise.

In matrix form:

$$P_{ij}^{n+m} = (P^n P^m)_{ij} = \sum_{k \in S} (P^n)_{ik} (P^m)_{kj}$$

$$\pi^{(n)} = \pi^{(n-1)} P$$

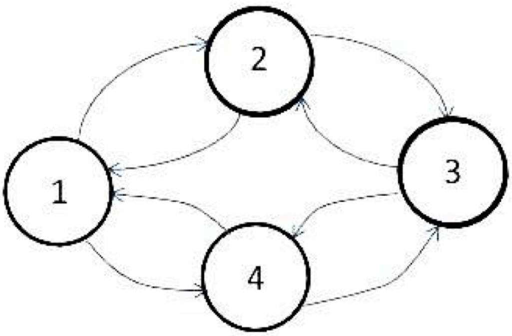
$$\pi^{(n)} = \sum_{i \in S} p_{ij}^{(n)} \pi_i^{(0)}$$

Classification of states

- A state j is accessible from state i if $p_{ij}^{(n)} > 0$ for some $n \geq 0$.
- State i and j communicate if both j is accessible from i and i is accessible from j.
- Two states that communicate are said to belong to the same equivalence class, and the state space S is divided into a certain number of such classes.
- The Markov chain is said to be irreducible if there is only one equivalence class (i.e. all states communicate with each other).
- A state i is absorbing if $p_{ii} = 1$.
- A state i is periodic with period d if d is the smallest integer such that $p_{ii}^{(n)} = 0$ for all n which are not multiples of d.
- In case $d = 1$, the state is said to be aperiodic.

Example

The Markov chain whose transition graph is given by is an irreducible Markov chain, periodic with period 2.



Recurrent and transient states

- Let us also define $f_i = P(X \text{ ever returns to } i | X_0 = i)$. A state i is said to be recurrent if $f_i = 1$ or transient if $f_i < 1$.
- It can be shown that all states in a given class are either recurrent or transient.
- In Example musical concert, the class "dancing", "at a concert", "at the bar" is transient (as there is a positive probability to leave the class and never come back) and the class "back home" is obviously recurrent.

$$P = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 1/2 & 0 & 1/2 & 0 \\ 1/4 & 1/4 & 1/4 & 1/4 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

- Proposition:
  State i is recurrent if and only if $\sum_{n\geq 1} p_{ii}^{(n)} = \infty$.
  State i is transient if and only if $\sum_{n\geq 1} p_{ii}^{(n)} < \infty$.

- Proof. Let T_i be the first time the chain X returns to state i $f_i = P(T_i < \infty | X_0 = i)$. Let N_i be the number of times that the chain returns to state i. Then

$$\begin{aligned} P(N_i < \infty | X_0 = i) &= \sum_{n \geq 1} P(X_n = i, X_m \neq i, \forall m > n | X_0 = i) \\ &= \sum_{n \geq 1} P(X_m \neq i, \forall m > n | X_n = i, X_0 = i) P(X_n = i | X_0 = i) \end{aligned}$$

As X is a time-homogeneous Markov chain, we have

$$P(X_m \neq i, \forall m > n | X_n = i, X_0 = i) = P(X_m \neq i, \forall m > n | X_n = i)$$

$$= P(X_m \neq i, \forall m > 0 | X_0 = i)$$

Therefore,

$$\begin{aligned} P(N_i < \infty | X_0 = i) &= P(X_m \neq i, \forall m > 0 | X_0 = i) \sum_{n \geq 1} P(X_n = i | X_0 = i) \\ &= P(T_i = \infty | X_0 = i) \sum_{i \geq 1} p_{ii}^{(n)} = (1 - f_i) \sum_{n \geq 1} p_{ii}^{(n)} \end{aligned}$$

- If i is recurrent, then $1 - f_i = 0$. We have $P(N_i < \infty | X_0 = i) = 0$. This in turn implies
$$P(N_i = \infty | X_0 = i) = 1, \text{so } E(N_i | X_0 = i) = \infty.$$
As $N_i = \sum_{n \geq 1} 1_{\{X_n = i\}}$, we have
$$\infty = E(N_i | X_0 = i) = \sum_{n \geq 1} E(1_{\{X_n = i\}} | X_0 = i)$$
$$= \sum_{n \geq 1} P(X_n = i | X_0 = i) = \sum_{n \geq 1} p_{ii}^{(n)}$$
- If i is transient, then $1 - f_i > 0$. As $P(N_i = \infty | X_0 = i) \leq 1$, we obtain
$$\sum_{n \geq 1} p_{ii}^{(n)} (1 - f_i) \leq 1, \sum_{n \geq 1} p_{ii}^{(n)} < \infty.$$

Stationary and limiting distributions

- A distribution $\pi^* = (\pi_i^*, i \in S)$ is said to be a stationary distribution for the Markov chain $(X_n, n \geq 0)$ if

$$\pi^* = \pi^* P, i.e. \pi_j^* = \sum_{i \in S} \pi_i^* \cdot p_{ij}, \forall j \in S$$

- π^* does not necessarily exist, nor is it necessarily unique.
- If π^* exists and is unique, then π_i^* can always be interpreted as the average proportion of time spent by the chain X in state i. $E(T_i | X_0 = i) = 1/\pi_i^*$, where $T_i = inf\{n \geq 0 : X_n = i\}$ is the first time the chain comes back to state i.
- If $\pi^{(0)} = \pi^*$,then $\pi^{(1)} = \pi^* P = \pi^*$;likewise,$\pi^{(n)} = \pi^*$,$\forall n \geq 0$.

- A distribution $\pi^* = (\pi_i^*, i \in S)$ is said to be a limiting distribution for the Markov chain $(X_n, n \geq 0)$ if for every initial distribution $\pi^{(0)}$ of the chain, we have

$$\lim_{n\to\infty} \pi^{(n)} = \pi^*, \forall i \in S$$

- If π^* is a limiting distribution, then it is stationary. Indeed, for all $n \geq 0$, we always have $\pi^{(n+1)} = \pi^{(n)}P$. If $\lim_{n\to\infty} \pi^{(n)} = \pi^*$, then $\pi^* = \pi^* P$.
- A limiting distribution π^* does not necessarily exist, but if it exists, then it is unique.

- Theorem 1. Let $(X_n, n \geq 0)$ be an irreducible and aperiodic Markov chain. Let us assume that it admits a stationary distribution π^*. Then π^* is a limiting distribution, i.e. for any initial distribution $\pi^{(0)}$, $\lim_{n\to\infty} \pi_i^{(n)} = \pi_i^*, \forall i \in S$.
- Theorem 2. Let $(X_n, n \geq 0)$ be an irreducible and positive recurrent Markov chain. Then X admits a unique stationary distribution π^*.

- Definition. A (time-homogeneous) Markov chain $(X_n, n \geq 0)$ is said to be ergodic if it is irreducible, aperiodic and positive recurrent.
- Corollary. An ergodic Markov chain $(X_n, n \geq 0)$ admits a unique stationary distribution π^*. Moreover, this distribution is also a limiting distribution, i.e. $\lim_{n\to\infty} \pi^{(n)} = \pi^*, \forall i \in S$.

Proof

证：有限 Markov 链是遍历的，故存在一个正整数 m，使得对于状态空间中的任何状态 i,j 有 $p_{i,j}^{(\mathrm{m})} > 0$。下面证明对于转移 M，有 $\lim_{n\to\infty} M^{(\mathrm{n})} = \pi$。这里 π 是一个随机矩阵，且它的各行都相同，它的每行即是平稳分布。

1、先证明 m=1 的情形。

若 m=1，则由条件可得，$p_{i,j} \geq \varepsilon > 0$。令 $m_j(\mathrm{n}) = \min_i p_{i,j}^{(\mathrm{n})}$，$M_j(\mathrm{n}) = \max_i p_{i,j}^{(\mathrm{n})}$。

由 Chapman-Kolmogorov 方程可知，$p_{i,j}^{(\mathrm{n})} = \sum_k p_{i,\mathrm{k}} p_{\mathrm{k},j}^{(\mathrm{n-1})} \geq \sum_k p_{i,\mathrm{k}} m_j(\mathrm{n-1}) = m_j(\mathrm{n-1})$。

上式对于所有的 i 都成立，因此，$m_j(\mathrm{n}) \geq m_j(\mathrm{n-1})$，这说明 $m_j(\mathrm{n})$ 随着 n 的增加而增加。

同理可以说明 $M_j(\mathrm{n})$ 随着 n 的增加而减少，即 $M_j(\mathrm{n}) \leq M_j(\mathrm{n-1})$。由于，$m_j(\mathrm{n})$、$M_j(\mathrm{n})$ 都是有界序列，故它们的极限存在。下面只需证明这两个序列的极限相同。

设当 $i = i_0$ 时，经 n 步转移后到达最小值 $m_j(\mathrm{n})$，又设 $i = i_1$ 时，经 n-1 步转移后到达最

Proof

大值$M_j(\mathrm{n}-1)$，则 $m_j(\mathrm{n}) = p^{(\mathrm{n})}_{i_0,j} = \sum_k p_{i_0,\mathrm{k}} p^{(\mathrm{n}-1)}_{\mathrm{k},j}$

$$= \varepsilon p^{(\mathrm{n}-1)}_{\mathrm{i}_1,j} + (p_{\mathrm{i}_0,\mathrm{i}_1} - \varepsilon) p^{(\mathrm{n}-1)}_{\mathrm{i}_1,j} + \sum_{k \neq j} p_{\mathrm{i}_0,\mathrm{k}} p^{(\mathrm{n}-1)}_{\mathrm{k},j}$$

$$\geq \varepsilon M_j(\mathrm{n}-1) + [p_{\mathrm{i}_0,\mathrm{i}_1} - \varepsilon + \sum_{k \neq j} p_{\mathrm{i}_0,\mathrm{k}}] m_j(\mathrm{n}-1)$$

即 $m_j(\mathrm{n}) \geq \varepsilon M_j(\mathrm{n}-1) + (1-\varepsilon) m_j(\mathrm{n}-1)$。

同理可得，$M_j(\mathrm{n}) \leq \varepsilon m_j(\mathrm{n}-1) + (1-\varepsilon) M_j(\mathrm{n}-1)$。

上式两式相减，得 $M_j(\mathrm{n}) - m_j(\mathrm{n}) \leq (1-2\varepsilon)[M_j(\mathrm{n}-1) - m_j(\mathrm{n}-1)]$，递推可得，$M_j(\mathrm{n}) - m_j(\mathrm{n}) \leq (1-2\varepsilon)^{n-1}$。因此，$n \to \infty$时，$m_j(\mathrm{n})$、$M_j(\mathrm{n})$趋于同一极限。这就证明了 $\lim_{n\to\infty} M^{(\mathrm{n})} = \pi$。$\pi$是各行都相同的矩阵。

Proof

2、m>1 时，$\lim\limits_{n\to\infty}(M^{(\mathrm{m})})^{(\mathrm{n})}=\lim\limits_{n\to\infty}M^{(\mathrm{mn})}=\pi$。又设 k=1,2,3,…,m-1，则

$\lim\limits_{n\to\infty}M^{(\mathrm{mn+k})}=\lim\limits_{n\to\infty}M^{(\mathrm{mn})}M^{(\mathrm{k})}=M^{(\mathrm{k})}\pi$。因为在 $M^{(\mathrm{k})}$ 中各行之和为 1，且 π 中的任何一列的元素都相等，因此 $M^{(\mathrm{k})}\pi=\pi$，即 $\lim\limits_{n\to\infty}M^{(\mathrm{mn+k})}=\pi$。

3、下面说明 $\lim\limits_{n\to\infty}P(\xi_n=\mathrm{j})=\lim\limits_{n\to\infty}p_{i,j}^{(\mathrm{n})}=\pi_j$，即 $\lim\limits_{n\to\infty}P(\xi_n=\mathrm{j})$ 所取的值与初始状态的分布无关。$P(\xi_n=\mathrm{j})=\sum\limits_i P(\xi_n=\mathrm{j}|\xi_0=i)P(\xi_0=i)=\sum\limits_i p_{i,j}^{(\mathrm{n})}P(\xi_0=i)$，

故 $\lim\limits_{n\to\infty}P(\xi_n=\mathrm{j})=\lim\limits_{n\to\infty}\sum\limits_i p_{i,j}^{(\mathrm{n})}P(\xi_0=i)=\sum\limits_i \pi_j P(\xi_0=i)$

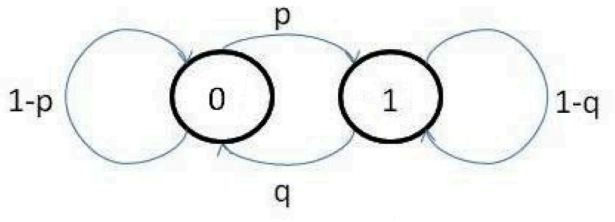
$$=\pi_j\sum_i P(\xi_0=i)=\lim_{n\to\infty}p_{i,j}^{(\mathrm{n})}。$$

4、证明其唯一性。

如果另有一矩阵 W 也满足 WM=W，且 W 的各行之和为 1.则

$W=WM=WM^{(2)}=\cdots=WM^{(\mathrm{n})}$。当 $n\to\infty$ 时，$W=W\pi$。W 中每行之和为 1，且 π 中每列元素都相等，从而 $W=W\pi=\pi$。唯一性得证。

Example: two-state Markov chain

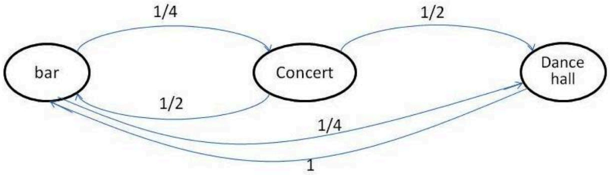


- Both $p, q > 0$, this chain is clearly irreducible, and as it is finite-state, it is also positive recurrent. It admits a stationary distribution.
- Since $\pi = \pi P$, we obtain

$$\pi_0 = \pi_0(1-p) + \pi_1 q, \pi_1 = \pi_0 p + \pi_1(1-q)$$

- π is a distribution, we must have $\pi_0 + \pi_1 = 1$ and $\pi_0, \pi_1 \geq 0$.
- Solving these equations, we obtain $\pi_0 = q/(p+q)$, $\pi_1 = p/(p+q)$.
- If $p + q < 2$, then the chain is also aperiodic and therefore ergodic, so $\pi = (q/(p+q), p/(p+q))$ is also a limiting distribution.

Example:music festival



It has the corresponding transition matrix:

$$P = \begin{pmatrix} 1/2 & 1/4 & 1/4 \\ 1/2 & 0 & 1/2 \\ 1 & 0 & 0 \end{pmatrix}$$

We can again easily see that the chain is ergodic. The computation of its stationary and limiting distribution gives

$$\pi^* = (8/13, 2/13, 3/13)$$

Example:simple symmetric random walk

Let us consider the simple symmetric random walk. This chain is irreducible, periodic with period 2 and all states are null recurrent. There does not exist a stationary distribution here.

Proposition: Let $(X_n, n \geq 0)$ be a finite-state irreducible Markov chain with state space $S = \{0, \cdots, N\}$ and let π^* be its unique stationary distribution. Then π^* is the uniform distribution if and only if the transition matrix P of the chain satisfies:

$$\sum_{i \in S} p_{ij} = 1, \forall j \in S.$$

Reversible Markov chains

Let $(X_n, n \geq 0)$ be a time-homogeneous Markov chain. Let us now consider this chain backwards, i.e. consider the process $(X_n, X_{n-1}, X_{n-2}, \cdots, X_1, X_0)$: this process turns out to be also a Markov chain (but not necessarily time-homogeneous). Indeed:

$$
\begin{aligned}
& P(X_n = j | X_{n+1} = i, X_{n+2} = k, X_{n+3} = l, \cdots) \\
= \quad & \frac{P(X_n = j, X_{n+1} = i, X_{n+2} = k, Xn + 3 = l, \cdots)}{P(X_{n+1} = i, X_{n+2} = k, X_{n+3} = l, \cdots)} \\
= \quad & \frac{P(X_{n+2} = k, X_{n+3} = l, \cdots, | X_{n+1} = i, X_n = j) P(X_{n+1} = j, X_n = j)}{P(X_{n+2} = k, X_{n+3} = l, \cdots, | X_{n+1} = i) P(X_{n+1} = i)} \\
= \quad & \frac{P(X_{n+2} = k, X_{n+3} = l, \cdots, | X_{n+1} = i)}{P(X_{n+2} = k, X_{n+3} = l, \cdots, | X_{n+1} = i)} P(X_n = j | X_{n+1} = i) \\
= \quad & P(X_n = j | X_{n+1} = i)
\end{aligned}
$$

Let us now compute the transition probabilities:

$$\begin{aligned} P(X_n = j | X_{n+1} = i) &= \frac{P(X_n = j, X_{n+1} = i)}{P(X_{n+1} = i)} \\ &= \frac{P(X_{n+1} = i | X_n = j) P(X_n = j)}{P(X_{n+1} = i)} \\ &= \frac{p_{ji} \pi_j^{(n)}}{\pi_i^{(n+1)}} \end{aligned}$$

The backward chain is not necessarily time-homogeneous.

- Let us now assume that the chain is irreducible and positive recurrent. Then it admits a unique stationary distribution π^*. Let us moreover assume that the initial distribution of the chain is the stationary distribution.

$$P(X_n = j | X_{n+1} = i) = \frac{p_{ji}\pi_j^*}{\pi_i^*} = \tilde{p}_{ij}$$

  The backward chain is time-homogeneous with transition probabilities $\tilde{p}_{ij}$.
- Definition: The chain X is said to be reversible if $\tilde{p}_{ij} = p_{ij}$, i.e. the transition probabilities of the forward and the backward chains are equal. In this case, the following detailed balance equation is satisfied:

$$\pi_i^* p_{ij} = \pi_j^* p_{ji}, \forall i, j \in S.$$

- If a distribution π^* satisfies the above detailed balance equation, then it is a stationary distribution. Indeed,

$$\sum_{i \in S} \pi_i^* pij = \sum_{i \in S} \pi_j^* p_{ji} = \pi_j^* \sum_{i \in S} p_{ji} = \pi_j^*, \forall j \in S$$

- In order to find the stationary distribution of a chain, solving the detailed balance equation is easier than solving the stationary distribution equation, but this works of course only if the chain is reversible.
- The detailed balance equation has the following interpretation: it says that in the Markov chain, the flow from state *i* to state *j* is equal to that from state *j* to state *i*.
- If the detailed balance equation is satisfied, then π^* is the uniform distribution if and only if *P* is a symmetric matrix.

Parameter estimation for Markov chains

- The elements of the training set $\{x_1, \cdots, x_n\}$, are assumed to be independent,
$$P(x_1, \cdots, x_n|\theta) = \Pi_j P(xj|\theta).$$
- MLE parameter estimation looks for θ which maximizes the above.
- WLOG, we consider there is only one Markov chain X with length L. We have
$$P(X|\theta) = \Pi_{j=1}^{L} p_{i_{j-1}, i_j}$$

Parameter estimation for Markov chains

- Let the transition probability matrix be P. $m_{kl} = |j : i_{j-1=k}, i_j = l|$. Then our optimization problem is formulated as:

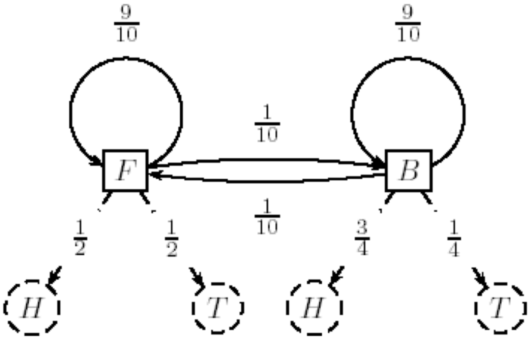
$$\max P(X|\theta) = \Pi_{k,l}^{L} p_{k,l}^{m_{kl}}$$

  s.t.

$$\sum_{l} p_{k,l} = 1, \forall k.$$

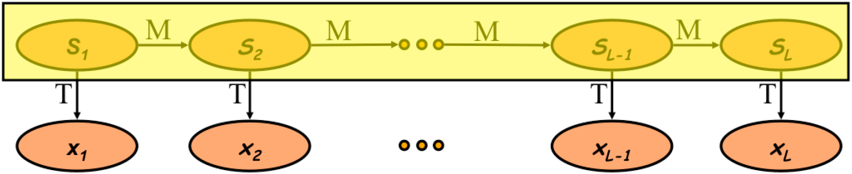
- By solving the maximization problem, we can get the MLE is given by:

$$p_{k,l} = \frac{m_{kl}}{\sum_{l'} m_{kl'}}$$



HMM model for the *Fair Bet Casino* Problem

Hidden Markov Model

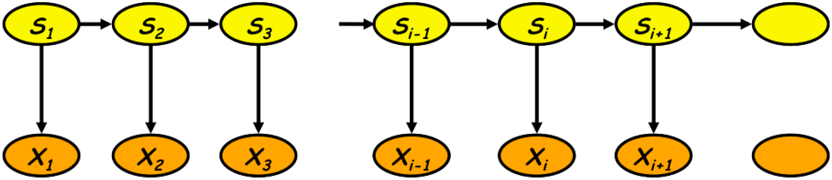


- Notations:
  Markov Chain transition probabilities: $P(S_{i+1} = t | S_i = s) = a_{st}$
  Emission probabilities: $P(X_i = b | S_i = s) = e_s(b)$
- For Markov Chains we know:

$$P(S) = P(s_1, s_2, \cdots, s_L) = \Pi_{i=1}^{L} P(s_i | s_{i-1})$$

- What is $P(s, x) = P(s_1, \cdots, s_L; x_1, \cdots, x_L)$?

Hidden Markov Model



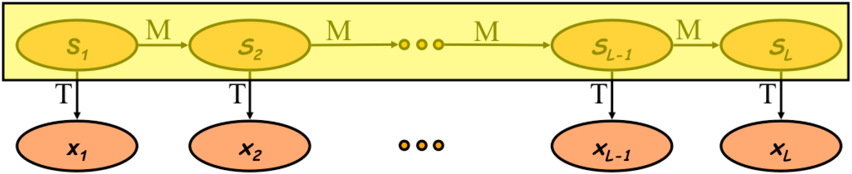
- Independence assumptions:

$$P(s_i|s_1,\cdots,s_{i-1},x_1,\cdots,x_{i-1}) = P(s_i|s_{i-1})$$

$$P(x_i|s_1,\cdots,s_i,x_1,\cdots,x_{i-1}) = P(x_i|s_i)$$

- $P(X_i = b|S_i = s) = e_s(b)$, means that the probability of x_i depends only on the probability of s_i.

Hidden Markov Model



- The joint distribution for the full chain:

$$P(s_1, x_1, s_2, x_2, \cdots, s_L, x_L) = P(s_1)P(x_1|s_1)\Pi_{i=2}^{L} P(s_i|s_{i-1})P(x_i|s_i)$$

Why "Hidden"?

- Observers can see the emitted symbols of an HMM but have no ability to know which state the HMM is currently in.
- Thus, the goal is to infer the most likely hidden states of an HMM based on the given sequence of emitted symbols.

HMM parameters

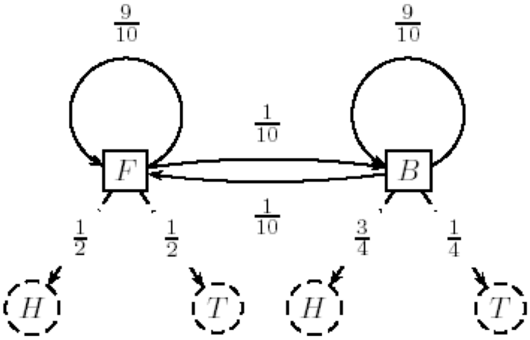
- Σ: set of emission characters.
  Example.:$\Sigma = \{H, T\}$ for coin tossing
  $\Sigma = \{1, 2, 3, 4, 5, 6\}$ for dice tossing
- Q: set of hidden states, each emitting symbols from Σ.
  $Q = \{F, B\}$ for coin tossing
- $A = (a_{kl})$: a $|Q| \times |Q|$ matrix of probability of changing from state k to state l.

$$a_{FF} = 0.9, a_{FB} = 0.1, a_{BF} = 0.1, a_{BB} = 0.9$$

- $E = (e_k(b))$: a $|Q|x|\Sigma|$ matrix of probability of emitting symbol b while being in state$k$.

$$e_F(H) = 1/2, e_F(T) = 1/2, e_B(T) = 1/4, e_B(H) = 3/4$$

Hidden Markov Model



HMM model for the *Fair Bet Casino* Problem

Three main problems in HMMs

- Evaluation: Given HMM parameters and observation sequence $\{x_1, x_2, \cdots, x_L\}$, find probability of the observed sequence $P(x_1, x_2, \cdots, x_L)$.
- Decoding: Given HMM parameters and observation sequence $\{x_1, x_2, \cdots, x_L\}$, find most probable sequence of hidden states:

$$\arg\max P(s_1, s_2, \cdots, s_L | x_1, x_2, \cdots, x_L)$$

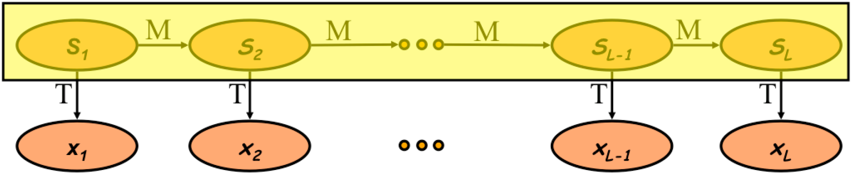
- Learning: Given HMM with unknown parameters and observation sequence, find parameters that maximize likelihood of observed data

$$\arg\max P(x_1, x_2, \cdots, x_L | \Theta)$$

HMM Algorithms

- Evaluation: What is the probability of the observed sequence? **Forward Algorithm**
- Decoding: What is the probability that the state s was loaded given the observed sequence? **Forward-Backward Algorithm**
  What is the most likely state sequence given the observed sequence? **Viterbi Algorithm**
- Learning: Under what parameterization is the observed sequence most probable? **Baum-Welch Algorithm (EM)**

Evaluation Problem



- Given HMM parameters: transition probability matrix A and emission probability matrix E, and observation sequence $\{x_1, x_2, \cdots, x_L\}$, find probability of observed sequence $P(X) = P(x_1, x_2, \cdots, x_L)$.
- $P(X) = \sum_S P(X, S)$. The summation taken over all state-paths s generating x. It requires K^L terms, where K is the number of different states.
- Instead: $P(x_1, x_2, \cdots, x_L) = \sum_k P(x_1, x_2, \cdots, x_L, S_L = k)$

Forward algorithm for computing P(x)

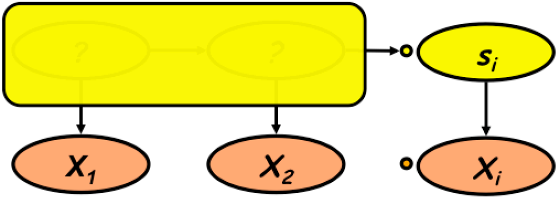
- Compute $P(x_1, x_2, \cdots, x_L, S_L = k)$ recursively.
- For $i = 1, \cdots, L$ and for each state l, compute:

$$f_l(i) = P(x_1, \cdots, x_i; s_i = l),$$

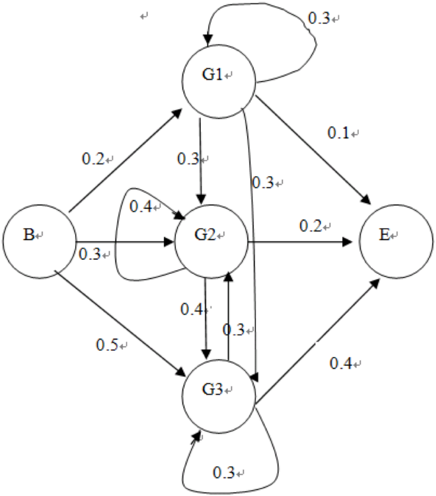
the probability of all the paths which emit $(x_1, \cdots, x_i)$ and end in state $s_i = l$.

- Use the recursive formula:

$$f_l(i) = e_l(x_i) \sum_k f_k(i-1) \cdot a_{kl}$$



Example



$$e_1(A) = 0.5, e_1(B) = 0.5$$
$$e_2(A) = 0.1, e_2(B) = 0.9$$
$$e_3(A) = 0.9, e_3(B) = 0.1$$

- Let $X = AAB$, compute $f_3(2)$.

Example

- Let $X = AAB$, compute $f_3(2)$.

$$
\begin{aligned}
f_1(1) &= 0.5 \times 0.2 = 0.1 \\
f_2(1) &= 0.1 \times 0.3 = 0.03 \\
f_3(1) &= 0.9 \times 0.5 = 0.45 \\
f_1(2) &= 0.5 \times 0.1 \times 0.3 = 0.015 \\
f_2(2) &= 0.1 \times (0.1 \times 0.3 + 0.03 \times 0.4 + 0.45 \times 0.3) = 0.0177 \\
f_3(2) &= 0.9 \times (0.1 \times 0.3 + 0.03 \times 0.4 + 0.45 \times 0.3) = 0.1593
\end{aligned}
$$

Decoding problem 1

- Problem: Given HMM parameters: transition prbability matrix A and emission probability matrix E, and observation sequence $\{x_1, x_2, \cdots, x_L\}$, compute for each $i = 1, \cdots, L$ and for each state k the probability that $s_i = k$.

$$P(s_i|x_1, x_2, \cdots, x_L) = \frac{P(s_i, x_1, x_2, \cdots, x_L)}{P(x_1, x_2, \cdots, x_L)}$$

- Decompose the computation:

$$\begin{aligned} P(x_1, \cdots, x_L, s_i) &= P(x_1, \cdots, x_i, s_i)P(x_{i+1}, \cdots, x_L|x_1, \cdots, x_i, s_i) \\ &= P(x_1, \cdots, x_i, s_i)P(x_{i+1}, \cdots, x_L|s_i) \\ &= f_{s_i}(i) \cdot b_{s_i}(i) \\ &= F(s_i)B(s_i) \end{aligned}$$

The backward algorithm

- Compute $B(s_i) = P(x_{i+1}, \cdots, x_L | s_i)$ for $i = L-1, \cdots, 1$ (namely, considering evidence after time slot i).
- First step, step $L-1$: Compute $B(s_{L-1})$.

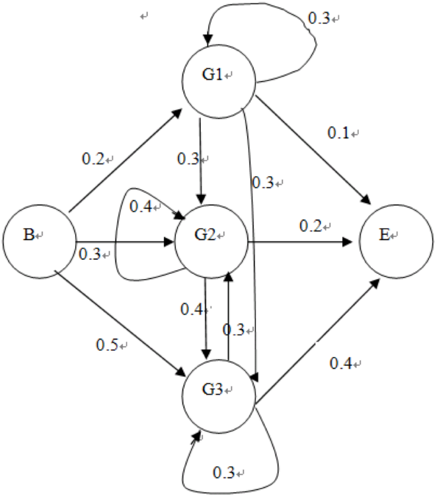
$$P(x_L | s_{L-1}) = \sum_{s_L} P(x_L, s_L | s_{L-1}) = \sum_{s_L} P(s_L | s_{L-1}) P(x_L | s_L)$$

- step i: compute $B(s_i)$ from $B(s_{i+1})$:

$$P(x_{i+1}, \cdots, x_L | s_i) = \sum_{s_{i+1}} P(s_{i+1} | s_i) P(x_{i+1} | s_{i+1}) P(x_{i+2}, \cdots, x_L | s_{i+1})$$

$$B(s_i) = \sum_{s_{i+1}} P(s_{i+1} | s_i) P(x_{i+1} | s_{i+1}) B(s_{i+1})$$

Example



$$e_1(A) = 0.5, e_1(B) = 0.5$$
$$e_2(A) = 0.1, e_2(B) = 0.9$$
$$e_3(A) = 0.9, e_3(B) = 0.1$$

- Let $X = AAB$, compute $b_3(2)$.

- Let $x = AAB$, compute $b_3(2)$.

$$b_1(3) = 0.1$$
$$b_2(3) = 0.2$$
$$b_3(3) = 0.4$$
$$b_1(2) = 0.3 \times 0.5 \times 0.1 + 0.3 \times 0.9 \times 0.2 + 0.3 \times 0.1 \times 0.4 = 0.081$$
$$b_2(2) = 0.4 \times 0.9 \times 0.2 + 0.4 \times 0.1 \times 0.4 = 0.088$$
$$b_3(2) = 0.3 \times 0.9 \times 0.2 + 0.3 \times 0.1 \times 0.4 = 0.066$$
$$b_1(1) = 0.3 \times 0.5 \times 0.081 + 0.3 \times 0.1 \times 0.088 + 0.3 \times 0.9 \times 0.066 = 0.03261$$
$$b_2(1) = 0.4 \times 0.1 \times 0.088 \times 0.4 \times 0.9 \times 0.066 = 0.02728$$
$$b_3(1) = 0.3 \times 0.1 \times 0.088 + 0.3 \times 0.9 \times 0.066 = 0.02046$$

Most likely state vs. Most likely sequence

- Most likely state assignment at time i

$$\arg\max P(S_i = k | x_1, x_2, \cdots, x_L)$$

  E.g. Which die was most likely used by the casino in the third roll given the observed sequence?

- Most likely assignment of state sequence

$$\arg\max_{S_i} P(S_i, i = 1, \cdots, L | x_1, x_2, \cdots, x_L)$$

  E.g. What was the most likely state sequence of die rolls used by the casino given the observed sequence?

- Not the same solution !

Decoding problem 2

- Problem: Given HMM parameters: transition prbability matrix A and emission probability matrix E, and observation sequence $\{x_1, x_2, \cdots, x_L\}$, find most likely assignment of state sequence.
-

$$
\begin{aligned}
&\arg\max_{(s_1,s_2,\cdots,s_L)} P(s_1, s_2, \cdots, s_L | x_1, x_2, \cdots, x_L) \\
&= \arg\max_{(s_1,s_2,\cdots,s_L)} P(s_1, s_2, \cdots, s_L, x_1, x_2, \cdots, x_L) \\
&= \arg\max_k \max_{(s_1,s_2,\cdots,s_{L-1})} P(s_1, s_2, \cdots, s_{L-1}, s_L = k, x_1, x_2, \cdots, x_L) \\
&= \arg\max_k v_k(L)
\end{aligned}
$$

Viterbi algorithm

- Compute probability $v_k(i)$ recursively over i.
-

$$
\begin{aligned}
v_k(i) &= \max_{s_1, s_2, \cdots, s_{i-1}} P(s_i = k, s_1, s_2, \cdots, s_{i-1}, x_1, x_2, \cdots, x_i) \\
&= P(x_i | s_i = k) \max_l P(s_i = k | s_{i-1} = l) v_l(i-1)
\end{aligned}
$$

Viterbi algorithm

- Initialization: $v_0(0) = 1$, $v_k(0) = 0$ for $k > 0$.
- For $i = 1$ to L do for each state l:

$$v_l(i) = e_l(x_i) \max_k v_k(i-1) a_{kl}$$

- Termination:

$$\max_{(s_1, s_2, \cdots, s_L)} P(s_1, s_2, \cdots, s_L, x_1, x_2, \cdots, x_L) = \max_k v_k(L)$$

- Trace back: $s_L = \arg\max_k v_k(L)$,
  $S_{i-1} = \arg\max_k P(s_i | s_{i-1} = k) v_k(i-1)$

Learning problem

- Given HMM with unknown parameters Θ and observation sequence $\{x_1, \cdots, x_L\}$, find parameters that maximize likelihood of observed data.

$$\arg\max P(x_1, \cdots, x_L | \Theta)$$

  But likelihood doesn't factorize since observations are not i.i.d.
- Hidden variables: state sequence $\{s_1, s_2, \cdots, s_L\}$.
- EM (Baum-Welch) Algorithm:
  E-step: Fix parameters, find expected state assignments
  M-step: Fix expected state assignments, update parameters

EM

- Expectation step (E-step): Calculate the expected value of the log likelihood function, with respect to the conditional distribution of $\mathbf{Z}$ given $\mathbf{X}$ under the current estimate of the parameters $\boldsymbol{\theta}^{(t)}$:

$$Q(\boldsymbol{\theta}|\boldsymbol{\theta}^{(t)}) = \mathrm{E}_{\mathbf{Z}|\mathbf{X},\boldsymbol{\theta}^{(t)}}\left[\log L(\boldsymbol{\theta};\mathbf{X},\mathbf{Z})\right]$$

- Maximization step (M-step): Find the parameter that maximizes this quantity:

$$\boldsymbol{\theta}^{(t+1)} = \underset{\boldsymbol{\theta}}{\arg\max}\ Q(\boldsymbol{\theta}|\boldsymbol{\theta}^{(t)})$$

E-Step:

$$
\begin{aligned}
& Q(\theta|\theta^t) \\
= & \sum_{s\in S} P(s|X,\theta^t)\log P(s,X|\theta) \\
= & \sum_{s\in S} P(s|X,\theta^t)\log(\pi_{s_1}\Pi_{t=1}^{T} a_{s_{t-1}s_t} e_{s_t}(x_t)) \\
= & \sum_{s\in S} P(s|X,\theta^t)\log \pi_{s_1} + \sum_{s\in S} P(s|X,\theta^t)\sum_{t=1}^{T}\log a_{s_{t-1}s_t} + \sum_{s\in S} P(s|X,\theta^t)\sum_{t=1}^{T}\log e_{s_t}(x_t)
\end{aligned} \tag{1}
$$

M-Step: The first term in Eqn. 1 becomes

$$\sum_{s \in S} P(s|X, \theta^t) \log \pi_1 = \sum_{i=1}^{N} P(S_1 = i|X, \theta^t) \log \pi_{1i}$$

By settiing its derivative equal to zero and using the constraint $\sum_{i=1}^{N} \pi_{1i} = 1$, we get:

$$\pi_{1i} = P(S_1 = i|X, \theta^t)$$

The second term in Eqn.1 becomes:

$$\sum_{s \in S} P(s|X, \theta^t) \sum_{t=1}^{T} \log a_{s_{t-1} s_t} = \sum_{i=1}^{N} \sum_{j=1}^{N} \sum_{t=1}^{T} P(s_{t-1} = i, s_t = j | X, \theta^t) \log a_{ij}$$

Use a Lagranger multiplier with the constraint $\sum_{j=1}^{N} a_{ij} = 1$, we have

$$a_{ij} = \frac{\sum_{t=1}^{T} P(s_{t-1} = i, s_t = j | X, \theta^t)}{\sum_{t=1}^{T} P(s_{t-1} = i | X, \theta^t)}$$

$$P(s_{i-1}=k, s_i=l|X,\theta)=\frac{f_k(i-1)a_{kl}e_l(x_i)b_l(i)}{P(X|\theta)},$$

where $f_k(i-1), b_l(i)$ are forward, backward algorithms for x under θ.

$$P(x_1,\cdots,x_L,s_{i-1}=k,s_i=l)$$

$$=P(x_1,\cdots,x_{i-1},s_{i-1}=k)a_{kl}e_k(x_i)P(x_{i+1},\cdots,x_L|s_i=l)$$

The third term in Eqn.1 becomes

$$\sum_{s \in S} P(s|X, \theta^t)(\sum_{t=1}^{T} \log e_{s_t}(x_t)) = \sum_{i=1}^{N} \sum_{t=1}^{T} P(s_t = i|X, \theta^t) \log e_i(x_t)$$

Similarly, by using a Lagrange multiplier with constraint $\sum_{j=1}^{L} e_i(j) = 1$, we get

$$e_i(k) = \frac{\sum_{t=1}^{T} P(s_t = i|X, \theta^t) \delta_{s_t, v_k}}{\sum_{t=1}^{T} P(s_t = i|X, \theta^t)}.$$

From another point of view. Here we assume there are n observed sequences. x^j denotes the j-th sequence.

- Step 1:For each pair (k, l), compute the expected number of state transitions from k to l:

$$
\begin{aligned}
A_{kl} &= \sum_{j=1}^{n} \frac{1}{P(x^j)} \sum_{i=1}^{L} P(x^j, s_{i-1} = k, s_i = l) \\
&= \sum_{j=1}^{n} \frac{1}{P(x^j)} \sum_{i=1}^{L} f_k^j(i-1) a_{kl}^j e_l^j(x_i) b_l^j(i)
\end{aligned}
$$

- Step 2: For each state k and each symbol b, compute the expected number of emissions of b from k:

$$
E_k(b) = \sum_{j=1}^{n} \frac{1}{P(x^j)} \sum_{i, x_i^j = b} f_k^j(i) b_k^j(i)
$$

- Step 3: Use the A_{kl}'s, $E_k(b)$'s to compute the new values of a_{kl} and $e_k(b)$. These values define Θ.

$$a_{kl} = \frac{A_{kl}}{\sum_{l'} A_{kl'}}, e_k(b) = \frac{E_k(b)}{\sum_{b'} E_k(b')}$$

- This procedure is iterated, until some convergence criterion is met.