# Hidden Markov Models 

Bartek Wilczyński

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## Materiały do dzisiejszego wykładu

- Do dzisiejszego wykładu: http://www.mimuw.edu.pl/~dojer/wobm/hmm.pdf


## Markov Models

- The model consists of a state space $Q \neq \emptyset$ (for our purposes $Q$ is finite)
- and a transition probability matrix $p_{i j}$ where $i, j \in Q$
- The model has no memory, the probability of moving from state $i$ to $j$ depends only on the state $i$.
- multiplying the matrix $P$, we can compute the change of the probability distribution as the model "steps" forward
- We are usually interested in stationary distributions $\pi$, such that $\pi \cdot P=P$

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Hidden Markov Model

image (c) wikipedia

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## Hidden Markov Model - trajectory


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## Hidden Markov Model - example


image (c) wikipedia

## Reconstructing HMM trajectories

For any trajectory $\pi$, we can calculate the probability of emiting $S$

$$
P(S, \pi)=\prod_{t=0}^{n-1} e_{\pi(t+1)}(S(t+1)) \cdot p_{\pi(t), \pi(t+1)}
$$

Can we find the optimal trajectory $\pi$, given $S$ ?

$$
P\left(S, \pi_{*}\right)=\max \left\{P(S, \pi)\left|\pi \in Q^{*},|\pi|=|S|\right\} .\right.
$$

## Viterbi algorithm

We can use dynamic programming, filling in the $v(i, k)$ matrix

$$
v(i, k)=\max \left\{P(S[1 . i], \pi) \mid \pi \in Q^{i}, \quad \pi(i)=k\right\} .
$$

with the initial condition:

$$
v(0, k)= \begin{cases}1 & \text { gdy } k=k_{0} \\ 0 & \text { gdy } k \neq k_{0}\end{cases}
$$

and step function:

$$
v(i, k)=e_{k}(S(i)) \cdot \max _{l \in Q}\left[v(i-1, l) \cdot p_{l, k}\right] .
$$

To finally read out the seeked probability:

$$
P\left(S, \pi_{*}\right)=\max _{k \in Q}[v(|S|, k)]
$$

## Estimating emission probabilities

Now, we can calculate the probability of emitting $S$, over all possible trajectories, with the Forward-method. The initial step is as follows:

$$
f(0, k)= \begin{cases}1 & \text { gdy } k=k_{0} \\ 0 & \text { gdy } k \neq k_{0}\end{cases}
$$

Then, we make similar steps:

$$
f(i, k)=e_{k}(S(i)) \cdot \sum_{l \in Q} f(i-1, l) \cdot p_{l, k}
$$

and finally we can calculate the total probability at the end:

$$
P(S)=\sum_{k \in Q} f(|S|, k)
$$

The same works backwards:

$$
b(i, k)=\sum_{l \in Q} p_{k, l} \cdot e_{l}(S(i+1)) \cdot b(i+1, l)
$$

## Estimating emission probabilities

Putting it together, probability of being in state $k$ at step $i$, given $S$ :

$$
P(\pi(i)=k \mid S)=\frac{P(\pi(i)=k \& S)}{P(S)}=\frac{f(i, k) \cdot b(i, k)}{P(S)} .
$$

## emission probabilities

Estimate of the Emission matrix:

$$
e_{k}(x)=\frac{E_{k}(x)}{\sum_{y \in \Sigma} E_{k}(y)}
$$

Can be calculated using $f$ and $b$

$$
E_{k}(x)=\sum_{j=1}^{n} \sum_{i \in I_{j}(x)} \frac{f_{\mathcal{M}}^{(j)}(i, k) \cdot b_{\mathcal{M}}^{(j)}(i, k)}{P_{\mathcal{M}}\left(S_{j}\right)}
$$

## Calculating probabilities

Similarly the transition matrix:

$$
p_{k, l}=\frac{P_{k, l}}{\sum_{q \in Q} P_{k, q}}
$$

depends on $f$ and $b$

$$
P_{k, l}=\sum_{j=1}^{n} \sum_{i=1}^{\left|S_{j}\right|} \frac{f_{\mathcal{M}}^{(j)}(i, k) \cdot p_{k, l}^{\mathcal{M}} \cdot e_{l}^{\mathcal{M}}\left(S_{j}(i+1)\right) \cdot b_{\mathcal{M}}^{(j)}(i+1, l)}{P_{\mathcal{M}}\left(S_{j}\right)} .
$$

## Baum-Welch algorithm

- Suppose, we only know the word $S$ and the sets $Q$ and $\Sigma$. Can we estimate both $p_{i j}$ and $e_{i j}$ ?
- We can start with random $p_{i j}, e_{i j}$ and iteratively proceed as follows:
- Calculate the estimates of being in each of states at each step using $f, b$ and current estimates of $e, p$.
- Find the optimal $e, p$, given current $e, p, f, b$
- This is an example of a known procedure called Expectation-Maximization
- It converges to a local optimum of the likelihood, because at every iteration, the likelihood cannot be decreased.


## Extensions and applications

- We will discuss it in more depth next week, but the HMM model is very useful in describing sequence alignments and so-called sequence profiles
- It is relatively easy to extend this model for arbitrary emissions (e.g. Gaussian or multinomial), not necessarily from a discrete space of symbols. This is frequently used for modelling functional genomics data
- It is also quite a good model for segmentation of chromosomes based on different measurements along the genome

