Dynamic Approaches: The Hidden Markov Model

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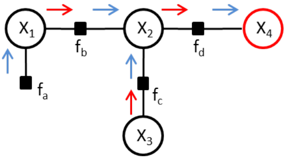
Machine Learning: Neural Networks and Advanced Models (AA2)

Inference as Message Passing

How to infer the distribution $P(\mathbf{X}_{unk}|\mathbf{X}_{obs})$ of a number of random variables $\mathbf{X}_{unk}$ in the graphical model, given the observed values of other variables $\mathbf{X}_{obs}$



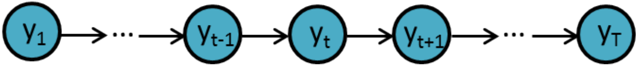
Directed and undirected models of fixed structure

- Exact inference
  - Passing messages (vectors of information) on the structure of the graphical model following a propagation direction
  - Works for chains, trees and can be used in (some) graphs
- Approximated inference can use approximations of the distribution (variational) or can estimate its expectation using examples (sampling)

Today's Lecture

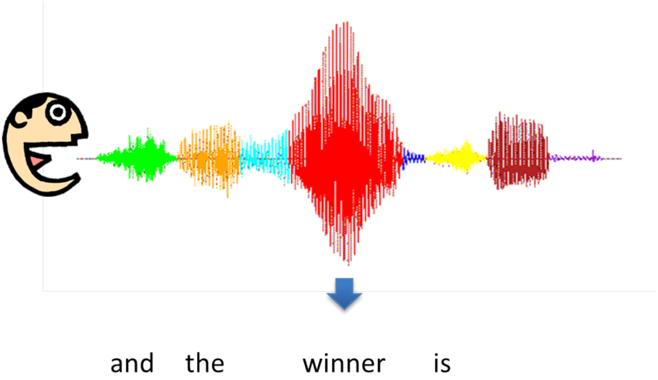
- Exact inference on a chain with observed and unobserved variables
- A probabilistic model for sequences: Hidden Markov Models (HMMs)
- Using inference to learn: the Expectation-Maximization algorithm for HMMs
- Graphical models with varying structure: Dynamic Bayesian Networks
- Application examples

Sequences

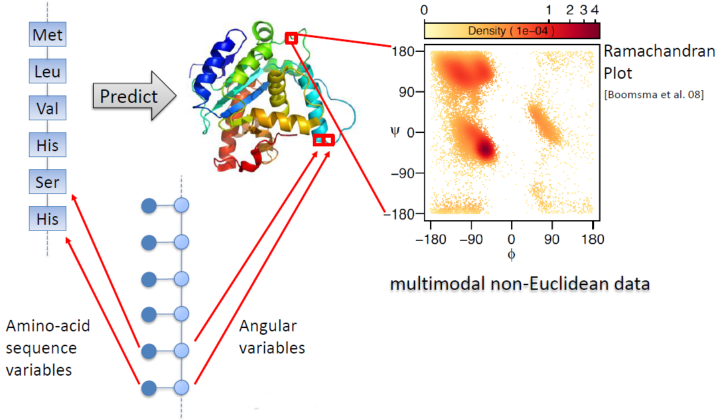


- A sequence $\mathbf{y}$ is a collection of observations y_t where t represent the position of the element according to a (complete) order (e.g. time)
- Reference population is a set of i.i.d sequences $\mathbf{y}^1, \ldots, \mathbf{y}^N$
- Different sequences $\mathbf{y}^1, \ldots, \mathbf{y}^N$ generally have different lengths $T^1, \ldots, T^N$

Sequences in Speech Processing



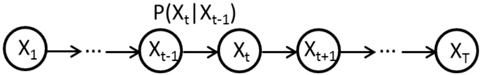
Sequences in Biology



Markov Chain

First-Order Markov Chain

Directed graphical model for sequences s.t. element X_t only depends on its predecessor in the sequence



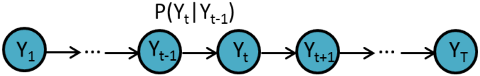
- Joint probability factorizes as

$$P(\mathbf{X}) = P(X_1, \dots, X_T) = P(X_1) \prod_{t=2}^{T} P(X_t | X_{t-1})$$

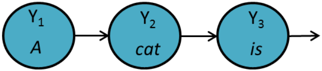
- $P(X_t|X_{t-1})$ is the transition distribution; $P(X_1)$ is the prior distribution
- General form: an L-th order Markov chain is such that X_t depends on L predecessors

Observed Markov Chains

Can we use a Markov chain to model the relationship between observed elements in a sequence?



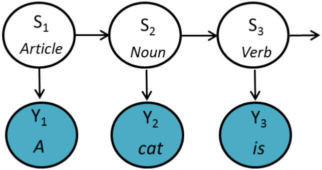
Of course yes, but...



Does it make sense to represent $P(is|cat)$?

Hidden Markov Model (HMM) (I)

Stochastic process where transition dynamics is disentangled from observations generated by the process

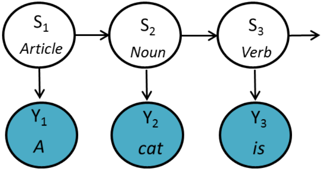


- State transition is an unobserved (hidden/latent) process characterized by the hidden state variables S_t
  - S_t are often discrete with value in $\{1, \dots, C\}$
  - Multinomial state transition and prior probability (stationariety assumption)

$$A_{ij} = P(S_t = i | S_{t-1} = j) \text{ and } \pi_i = P(S_t = i)$$

Hidden Markov Model (HMM) (II)

Stochastic process where transition dynamics is disentangled from observations generated by the process



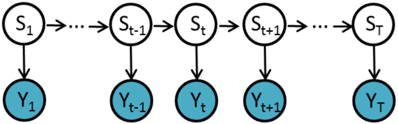
- Observations are generated by the emission distribution

$$b_i(y_t) = P(Y_t = y_t | S_t = i)$$

HMM Joint Probability Factorization

Discrete-state HMMs are parameterized by $\theta = (\pi, A, B)$ and the finite number of hidden states C

- State transition and prior distribution A and π
- Emission distribution B (or its parameters)

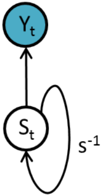


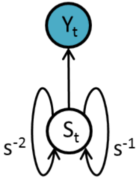
$$P(\mathbf{Y} = \mathbf{y}) = \sum_{\mathbf{s}} P(\mathbf{Y} = \mathbf{y}, \mathbf{S} = \mathbf{s})$$

$$= \sum_{s_1,\ldots,s_T} \left\{ P(S_1 = s_1) P(Y_1 = y_1 | S_1 = s_1) \prod_{t=2}^{T} P(S_t = s_t | S_{t-1} = s_{t-1}) P(Y_t = y_t | S_t = s_t) \right\}$$

HMMs as a Recursive Model

A graphical framework describing how contextual information is recursively encoded by both probabilistic and neural models





- Indicates that the hidden state S_t at time t is dependent on context information from
  - The previous time step s^{-1}
  - Two time steps earlier s^{-2}
  - ...
- When applying the recursive model to a sequence (unfolding), it generates the corresponding directed graphical model

3 Notable Inference Problems

Definition (Smoothing)

Given a model θ and an observed sequence $\mathbf{y}$, determine the distribution of the t-th hidden state $P(S_t|\mathbf{Y} = \mathbf{y}, \theta)$

Definition (Learning)

Given a dataset of N observed sequences $\mathcal{D} = \{\mathbf{y}^1, \dots, \mathbf{y}^N\}$ and the number of hidden states C, find the parameters π, A and B that maximize the probability of model $\theta = \{\pi, A, B\}$ having generated the sequences in $\mathcal{D}$

Definition (Optimal State Assignment)

Given a model θ and an observed sequence $\mathbf{y}$, find an optimal state assignment $\mathbf{s} = s_1^*, \dots, s_T^*$ for the hidden Markov chain

Forward-Backward Algorithm

Smoothing - How do we determine the posterior $P(S_t = i|\mathbf{y})$?

Exploit factorization

$$P(S_t = i|\mathbf{y}) \propto P(S_t = i, \mathbf{y}) = P(S_t = i, \mathbf{Y}_{1:t}, \mathbf{Y}_{t+1:T})$$
$$= P(S_t = i, \mathbf{Y}_{1:t}) P(\mathbf{Y}_{t+1:T} | S_t = i) = \alpha_t(i)\beta_t(i)$$

α-term computed as part of forward recursion ($\alpha_1(i) = b_i(y_1)\pi_i$)

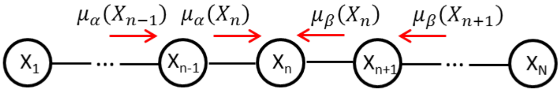
$$\alpha_t(i) = P(S_t = i, \mathbf{Y}_{1:t}) = b_i(y_t) \sum_{j=1}^{C} A_{ij}\alpha_{t-1}(j)$$

β-term computed as part of backward recursion ($\beta_T(i) = 1, \forall i$)

$$\beta_t(j) = P(\mathbf{Y}_{t+1:T} | S_t = j) = \sum_{i=1}^{C} b_i(y_{t+1})\beta_{t+1}(i)A_{ij}$$

Deja vu

Doesn't the Forward-Backward algorithm look strangely familiar?



- $\alpha_t \equiv \mu_\alpha(X_n) \rightarrow$ forward message

$$\underbrace{\mu_\alpha(X_n)}_{\alpha_t(i)} = \underbrace{\sum_{X_{n-1}}}_{\sum_{j=1}^{C}} \underbrace{\psi(X_{n-1}, X_n)}_{b_i(y_t)A_{ij}} \underbrace{\mu_\alpha(X_{n-1})}_{\alpha_{t-1}(j)}$$

- $\beta_t \equiv \mu_\beta(X_n) \rightarrow$ backward message

$$\underbrace{\mu_\beta(X_n)}_{\beta_t(j)} = \underbrace{\sum_{X_{n+1}}}_{\sum_{i=1}^{C}} \underbrace{\psi(X_n, X_{n+1})}_{b_i(y_{t+1})A_{ij}} \underbrace{\mu_\beta(X_{n+1})}_{\beta_{t+1}(i)}$$

Learning in HMM

Learning HMM parameters $\theta = (\pi, A, B)$ by maximum likelihood

$$
\begin{aligned}
\mathcal{L}(\theta) &= \log \prod_{n=1}^{N} P(\mathbf{Y}^n|\theta) \\
&= \log \prod_{n=1}^{N} \left\{ \sum_{s_1^n,\dots,s_{T_n}^n} P(S_1^n)P(Y_1^n|S_1^n) \prod_{t=2}^{T_n} P(S_t^n|S_{t-1}^n)P(Y_t^n|S_t^n) \right\}
\end{aligned}
$$

- How can we deal with the unobserved random variables S_t and the nasty summation in the log?
- Expectation-Maximization algorithm
  - Maximization of the complete likelihood $\mathcal{L}_c(\theta)$
  - Completed with indicator variables

$$
z_{ti}^n = \begin{cases} 1 \text{ if } n\text{-th chain is in state } i \text{ at time } t \\ 0 \text{ otherwise} \end{cases}
$$

Complete HMM Likelihood

Introduce indicator variables in $\mathcal{L}(\theta)$ together with model parameters $\theta = (\pi, A, B)$

$$\mathcal{L}_c(\theta) = \log P(\mathcal{X}, \mathcal{Z}|\theta) = \log \prod_{n=1}^{N} \left\{ \prod_{i=1}^{C} [P(S_1^n = i) P(Y_1^n | S_1^n = i)]^{z_{1i}^n} \right.$$

$$\left. \prod_{t=2}^{T_n} \prod_{i,j=1}^{C} P(S_t^n = i | S_{t-1}^n = j)^{z_{ti}^n z_{(t-1)j}^n} P(Y_t^n | S_t^n = i)^{z_{ti}^n} \right\}$$

$$= \sum_{n=1}^{N} \left\{ \sum_{i=1}^{C} z_{1i}^n \log \pi_i + \sum_{t=2}^{T_n} \sum_{i,j=1}^{C} z_{ti}^n z_{(t-1)j}^n \log A_{ij} + \sum_{t=1}^{T_n} \sum_{i=1}^{C} z_{ti}^n \log b_i(y_t^n) \right\}$$

Expectation-Maximization

A 2-step iterative algorithm for the maximization of complete likelihood $\mathcal{L}_c(\theta)$ w.r.t. model parameters θ

E-Step: Given the current estimate of the model parameters $\theta^{(t)}$, compute

$$Q^{(t+1)}(\theta|\theta^{(t)}) = E_{\mathcal{Z}|\mathcal{X},\theta^{(t)}}[\log P(\mathcal{X}, \mathcal{Z}|\theta)]$$

M-Step: Find the new estimate of the model parameters

$$\theta^{(t+1)} = \arg\max_{\theta} Q^{(t+1)}(\theta|\theta^{(t)})$$

Iterate 2 steps until $|\mathcal{L}_c(\theta)^{it} - \mathcal{L}_c(\theta)^{it-1}| < \epsilon$ (or stop if maximum number of iterations is reached)

E-Step (I)

Compute the expected value expectation of the complete log-likelihood w.r.t indicator variables z_{ti}^n assuming (estimated) parameters $\theta^t = (\pi^t, A^t, B^t)$ fixed at time t (i.e. constants)

$$Q^{(t+1)}(\theta|\theta^{(t)}) = E_{\mathcal{Z}|\mathcal{X},\theta^{(t)}}[\log P(\mathcal{X}, \mathcal{Z}|\theta)]$$

Expectation w.r.t a (discrete) random variable z is

$$E_z[Z] = \sum_z z \cdot P(Z = z)$$

To compute the conditional expectation $Q^{(t+1)}(\theta|\theta^{(t)})$ for the complete HMM log-likelihood we need to estimate

$$E_{\mathcal{Z}|\mathbf{Y},\theta^{(k)}}[z_{ti}] = P(S_t = i|\mathbf{y})$$

$$E_{\mathcal{Z}|\mathbf{Y},\theta^{(k)}}[z_{ti}z_{(t-1)j}] = P(S_t = i, S_{t-1} = j|\mathbf{Y})$$

E-Step (II)

We know how to compute the posteriors by the forward-backward algorithm!

$$\gamma_t(i) = P(S_t = i|\mathbf{Y}) = \frac{\alpha_t(i)\beta_t(i)}{\sum_{j=1}^{C} \alpha_t(j)\beta_t(j)}$$

$$\gamma_{t,t-1}(i,j) = P(S_t = i, S_{t-1} = j|\mathbf{Y}) = \frac{\alpha_{t-1}(j)A_{ij}b_i(y_t)\beta_t(i)}{\sum_{m,l=1}^{C} \alpha_{t-1}(m)A_{lm}b_l(y_t)\beta_t(l)}$$

M-Step (I)

Solve the optimization problem

$$\theta^{(t+1)} = \arg\max_{\theta} Q^{(t+1)}(\theta|\theta^{(t)})$$

using the information computed at the E-Step (the posteriors). How?

As usual

$$\frac{\partial Q^{(t+1)}(\theta|\theta^{(t)})}{\partial \theta}$$

where $\theta = (\pi, A, B)$ are now variables.

Attention

Parameters can be distributions $\Rightarrow$ need to preserve sum-to-one constraints (Lagrange Multipliers)

M-Step (II)

State distributions

$$A_{ij} = \frac{\sum_{n=1}^{N} \sum_{t=2}^{T^n} \gamma_{t,t-1}^{n}(i,j)}{\sum_{n=1}^{N} \sum_{t=2}^{T^n} \gamma_{t-1}^{n}(j)} \quad \text{and} \quad \pi_i = \frac{\sum_{n=1}^{N} \gamma_1^n(i)}{N}$$

Emission distribution (multinomial)

$$B_{ki} = \frac{\sum_{n=1}^{N} \sum_{t=1}^{T_n} \gamma_t^n(i)\delta(y_t = k)}{\sum_{n=1}^{N} \sum_{t=1}^{T_n} \gamma_t^n(i)}$$

where $\delta(\cdot)$ is the indicator function for emission symbols k

Decoding Problem

- Find the optimal hidden state assignement $\mathbf{s} = s_1^*, \ldots, s_T^*$ for an observed sequence $\mathbf{y}$ given a trained HMM
- No unique interpretation of the problem
  - Identify the single hidden states s_t that maximize the posterior
$$s_t^* = \arg \max_{i=1,\ldots,C} P(S_t = i|\mathbf{Y})$$
  - Find the most likely joint hidden state assignment
$$\mathbf{s}^* = \arg \max_{\mathbf{s}} P(\mathbf{Y}, \mathbf{S} = \mathbf{s})$$
- The last problem is addressed by the Viterbi algorithm

Viterbi Algorithm

An efficient dynamic programming algorithm based on a backward-forward recursion

An example of a max-product message passing algorithm

Recursive backward term

$$\epsilon_{t-1}(s_{t-1}) = \max_{s_t} P(Y_t|S_t = s_t)P(S_t = s_t|S_{t-1} = s_{t-1})\epsilon_t(s_t),$$

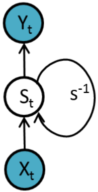
Root optimal state

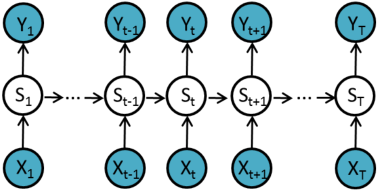
$$s_1^* = \arg\max_s P(Y_t|S_1 = s)P(S_1 = s_1)\epsilon_1(s).$$

Recursive forward optimal state

$$s_t^* = \arg\max_s P(Y_t|S_t = s)P(S_t = s|S_{t-1} = s_{t-1}^*)\epsilon_t(s).$$

Input-Output Hidden Markov Models

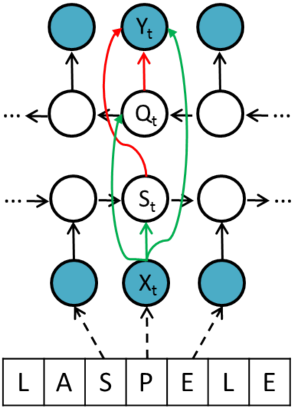




- Translate an input sequence into an output sequence (transduction)
- State transition and emissions depend on input observations (input-driven)
- Recursive model highlights analogy with recurrent neural networks

Bidirectional Input-driven Models

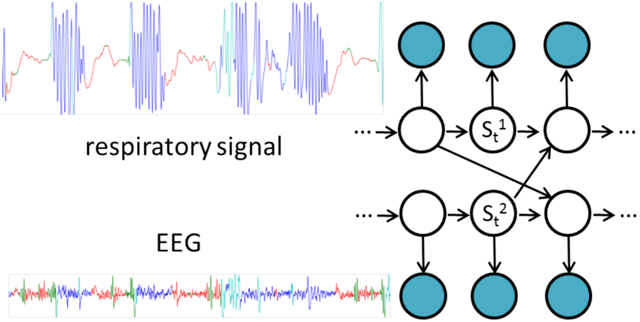
Remove causality assumption that current observation does not depend on the future and homogeneity assumption that an state transition is not dependent on the position in the sequence



- Structure and function of a region of DNA and protein sequences may depend on upstream and downstream information
- Hidden state transition distribution changes with the amino-acid sequence being fed in input

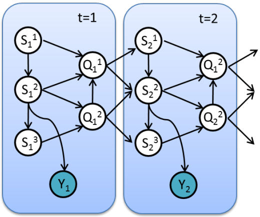
Coupled HMM

Describing interacting processes whose observations follow different dynamics while the underlying generative processes are interlaced

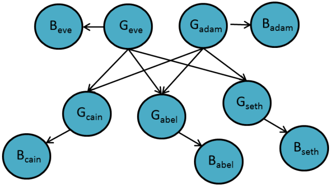


Dynamic Bayesian Networks

HMMs are a specific case of a class of directed models that represent dynamic processes and data with changing connectivity template



Hierarchical HMM



Structure changing information

Dynamic Bayesian Networks (DBN)

Graphical models whose structure changes to represent evolution across time and/or between different samples

Take Home Messages

- Hidden Markov Models
  - Hidden states used to realize an unobserved generative process for sequential data
  - A mixture model where selection of the next component is regulated by the transition distribution
  - Hidden states summarize (cluster) information on subsequences in the data
- Inference in HMMS
  - Forward-backward - Hidden state posterior estimation
  - Expectation-Maximization - HMM parameter learning
  - Viterbi - Most likely hidden state sequence
- Dynamic Bayesian Networks
  - A graphical model whose structure changes to reflect information with variable size and connectivity patterns
  - Suitable for modeling structured data (sequences, tree, ...)