Terminology, Representation and Basic Problems



The next three weeks

Hidden Markov models (HMMs):

- Wed 31/10: Terminology and basic algorithms.
- Fri 2/11: Implementing the basic algorithms.
- Wed 7/11: Implementing the basic algorithms, cont.

Selecting model parameters and training.

- Fri 9/11: Selecting model parameters and training, cont.
- Wed 14/11: Introduction to mandatory project.
- Fri 16/11: Extensions and applications.

We use Chapter 13 from Bishop's book "Pattern Recognition and Machine Learning". Rabiner's paper "A Tutorial on Hidden Markov Models [...]" might also be useful to read.

Blackboard and http://cs.au.dk/~cstorm/courses/ML_e18

What is machine learning?

Machine learning means different things to different people, and there is no general agreed upon core set of algorithms that must be learned.

For me, the core of machine learning is:

Building a mathematical model that captures some desired structure of the data that you are working on.

Training the model (i.e. set the parameters of the model) based on existing data to optimize it as well as we can.

Making predictions by using the model on new data.

Data – Observations

A sequence of observations from a finite and discrete set, e.g. measurements of weather patterns, daily values of stocks, the composition of DNA or proteins, or ...

$$\mathbf{X} = \mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N$$

Typical question/problem: How likely is a given **X**, i.e. p(**X**)?

We need a model that describes how to compute $p(\mathbf{X})$

Simple Models (1)

Observations are independent and identically distributed

$$\mathbf{x}_1$$
 \mathbf{x}_2 \mathbf{x}_3 \mathbf{x}_4 \cdots

$$p(\mathbf{x}_1,\ldots,\mathbf{x}_N) = \prod_{n=1}^N p(\mathbf{x}_n)$$

Too simplistic for realistic modelling of many phenomena

Simple Models (2)

The *n*'th observation in a chain of observations is influenced only by the *n*-1'th observation, i.e.

$$p(\mathbf{x}_n | \mathbf{x}_1, \dots, \mathbf{x}_{n-1}) = p(\mathbf{x}_n | \mathbf{x}_{n-1})$$

The chain of observations is a 1st-order Markov chain, and the probability of a sequence of *N* observations is

$$p(\mathbf{x}_1,\ldots,\mathbf{x}_N) = \prod_{n=1}^N p(\mathbf{x}_n | \mathbf{x}_1,\ldots,\mathbf{x}_{n-1}) = p(\mathbf{x}_1) \prod_{n=2}^N p(\mathbf{x}_n | \mathbf{x}_{n-1})$$



$$p(\mathbf{x}_n|\mathbf{x}_1,\ldots,\mathbf{x}_{n-1}) = p(\mathbf{x}_n|\mathbf{x}_{n-1})$$



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What if the *n*'th observation in a chain of observations is influenced by a corresponding hidden variable?

Latent values



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What if the *n*'th observation in a chain of observations is influenced The joint distribution

$$p(\mathbf{x}_1, \dots, \mathbf{x}_N, \mathbf{z}_1, \dots, \mathbf{z}_N) = p(\mathbf{z}_1) \left[\prod_{n=2}^N p(\mathbf{z}_n | \mathbf{z}_{n-1}) \right] \prod_{n=1}^N p(\mathbf{x}_n | \mathbf{z}_n)$$







Transition probabilities

Notation: In Bishop, the hidden variables \mathbf{z}_n are positional vectors, e.g. if $\mathbf{z}_n = (0,0,1)$ then the model in step *n* is in state *k*=3

Transition probabilities: If the hidden variables are discrete with *K* states, the conditional distribution $p(\mathbf{z}_n | \mathbf{z}_{n-1})$ is a $K \ge K$ table **A**, and the marginal distribution $p(\mathbf{z}_1)$ describing the initial state is a *K* vector **T**

The probability of going from state *j* to state *k* is:

$$A_{jk} \equiv p(z_{nk} = 1 | z_{n-1,j} = 1)$$

$$\sum_{k} A_{jk} = 1$$

The probability of state *k* being the initial state is:

$$\pi_k \equiv p(z_{1k} = 1)$$

$$\sum_k \pi_k = 1$$



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Emission probabilities

Emission probabilities: The conditional distributions of the observed variables $p(\mathbf{x}_n | \mathbf{z}_n)$ from a specific state

If the observed values \mathbf{x}_n are discrete (e.g. *D* symbols), the emission probabilities $\boldsymbol{\Phi}$ is a *K*x*D* table of probabilities which for each of the *K* states specifies the probability of emitting each observable ...

$$p(\mathbf{x}_n | \mathbf{z}_n, \phi) = \prod_{k=1}^{K} p(\mathbf{x}_n | \phi_k)^{z_{nk}}$$



Emission prob

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K

24=1).



HMM joint probability distribution

$$p(\mathbf{X}, \mathbf{Z} | \boldsymbol{\Theta}) = p(\mathbf{z}_1 | \pi) \left[\prod_{n=2}^{N} p(\mathbf{z}_n | \mathbf{z}_{n-1}, \mathbf{A}) \right] \prod_{n=1}^{N} p(\mathbf{x}_n | \mathbf{z}_n, \phi)$$





If A and **\phi** are the same for all *n* then the HMM is *homogeneous*

Example – 2-state HMM

Observable: {A, C, G, T}, States: {0,1}



Example – 7-state HMM

Observable: {A, C, G, T}, States: {0,1, 2, 3, 4, 5, 6}

Λ	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	0.00 0.00 0.00 1.00 0.00 0.00	$\begin{array}{cccccccccccccccccccccccccccccccccccc$
Α	0.00 0.00 0.00 0.10 0.90 0.00 0.00	π 0.00 φ	0.15 0.30 0.20 0.35



HMMs as a generative model

A HMM generates a sequence of observables by moving from latent state to latent state according to the transition probabilities and emitting an observable (from a discrete set of observables, i.e. a finite alphabet) from each latent state visited according to the emission probabilities of the state ...



A run follows a sequence of states:

HHLLH

And emits a sequence of symbols:



Computing P(X,Z)

$$p(\mathbf{X}, \mathbf{Z} | \boldsymbol{\Theta}) = p(\mathbf{z}_1 | \pi) \left[\prod_{n=2}^{N} p(\mathbf{z}_n | \mathbf{z}_{n-1}, \mathbf{A}) \right] \prod_{n=1}^{N} p(\mathbf{x}_n | \mathbf{z}_n, \phi)$$

```
def joint_prob(x, z):
    """
    Returns the joint probability of x and z
    """
    p = init_prob[z[0]] * emit_prob[z[0]][x[0]]
    for i in range(1, len(x)):
        p = p * trans_prob[z[i-1]][z[i]] * emit_prob[z[i]][x[i]]
        return p
```

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```
$ python hmm jointprob.py hmm-7-state.txt test seq100.txt
         > seq100
         p(x,z) = 1.8619524290102162e-65
def jo $ python hmm_jointprob.py hmm-7-state.txt test_seq200.txt
         > seq200
         p(x,z) = 1.6175774997005771e-122
         $ python hmm jointprob.py hmm-7-state.txt test seq300.txt
         > seq300
         p(x,z) = 3.0675430597843052e-183
         $ python hmm jointprob.py hmm-7-state.txt test seq400.txt
         > seq400
         p(x,z) = 4.860704144302979e-247
         $ python hmm jointprob.py hmm-7-state.txt test seq500.txt
         > seq500
         p(x,z) = 5.258724342206735e-306
         $ python hmm jointprob.py hmm-7-state.txt test_seq600.txt
         > seq600
         p(x,z) = 0.0
```

[x[i]]

Computing P(X,Z)

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                                                                               [x[i]]
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         p(x,z) = 5.258724342206735e-306
         $ python hmm jointprob.py hmm-7-state.txt test seq600.txt
         > seq600
         p(x, z) = 0.0
                            Should be >0 by construction of X and Z
```

Representing numbers

A floating point number *n* is represented as $n = f * 2^e$ cf. the IEEE-754 standard which specify the range of *f* and *e*



Item	Single precision	Double precision
Bits in sign	1	1
Bits in exponent	8	11
Bits in fraction	23	52
Bits, total	32	64
Exponent system	Excess †27	Excess 1023
Exponent range	-126 to +127	-1022 to +1023
Smallest normalized number	2-126	2-1022
Largest normalized number	approx. 2 ¹²⁸	approx. 2 ¹⁰²⁴
Decimal range	approx. 10-385 to 1038	approx. 10 ⁻³⁰⁸ to 10 ³⁰⁰
Smallest denormalized number	approx. 100-45	approx. 10 ⁻³²⁴

Figure B-5. Characteristics of IEEE filoating-point numbers.

See e.g. Appendix B in Tanenbaum's Structured Computer Organization for further details.

The problem – Too small numbers

For the simple HMM, the joint-probability $p(\mathbf{X}, \mathbf{Z})$ is

$$p(\mathbf{X}, \mathbf{Z}) = 1 \cdot \prod_{n=2}^{N} 1 \cdot \prod_{n=1}^{N} \frac{1}{2} = \left(\frac{1}{2}\right)^n = 2^{-n}$$

If n > 467 then 2^{-n} is smaller than 10^{-324} , i.e. cannot be represented



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No problem representing

 $\log p(\mathbf{X}, \mathbf{Z}) = -n$

as the decimal range is approx -10³⁰⁸ to 10³⁰⁸



A simple HMM

Solution: Compute log P(X,Z)

$$p(\mathbf{X}, \mathbf{Z} | \boldsymbol{\Theta}) = p(\mathbf{z}_1 | \pi) \left[\prod_{n=2}^{N} p(\mathbf{z}_n | \mathbf{z}_{n-1}, \mathbf{A}) \right] \prod_{n=1}^{N} p(\mathbf{x}_n | \mathbf{z}_n, \phi)$$

Use log $(XY) = \log X + \log Y$, and define log 0 to be -inf

$$\log p(\mathbf{X}, \mathbf{Z} | \boldsymbol{\Theta}) = \log p(\mathbf{z}_1 | \pi) + \sum_{n=2}^{N} \log p(\mathbf{z}_n | \mathbf{z}_{n-1}, \mathbf{A}) + \sum_{n=1}^{N} \log p(\mathbf{x}_n | \mathbf{z}_n, \phi)$$

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```
def log_joint_prob(self, x, z):
    """
    Returns the log transformed joint probability of x and z
    """
    logp = log(init_prob[z[0]]) + log(emit_prob[z[0]][x[0]])
    for i in range(1, len(x)):
        logp = logp + log(trans_prob[z[i-1]][z[i]]) + log(emit_prob[z[i]][x[i]])
    return logp
```

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[z[i]][x[i]])

```
$ python hmm log jointprob.py hmm-7-state.txt test seq100.txt
     log_joint > seq100
def
                  \log p(x,z) = -149.04640541441395
     111111
     Returns t $ python hmm_log_jointprob.py hmm-7-state.txt test seq200.txt
                  > seq200
     .....
                  \log p(x,z) = -280.43445168576596
     logp = lc
                  $ python hmm log jointprob.py hmm-7-state.txt test seq300.txt
     for i in
                  > seq300
          logp \log p(x,z) = -420.25219508298494
     return lo
                  $ python hmm log jointprob.py hmm-7-state.txt test seq400.txt
                  > seq400
                  \log p(x,z) = -567.1573346564519
                  $ python hmm log jointprob.py hmm-7-state.txt test seq500.txt
                  > seq500
                  \log p(x,z) = -702.9311499793356
                  $ python hmm log jointprob.py hmm-7-state.txt test seq600.txt
                  > seq600
                  \log p(x,z) = -842.0056730984585
```

Using HMMs

- Determine the likelihood of a sequence of observations.
- Find a plausible underlying explanation (or decoding) of a sequence of observations.

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$$p(\mathbf{X}|\mathbf{\Theta}) = \sum_{\mathbf{Z}} p(\mathbf{X}, \mathbf{Z}|\mathbf{\Theta})$$

The sum has K^N terms, but it turns out that it can be computed in $O(K^2N)$ time, but first we will consider **decoding**

Decoding using HMMs

Given a HMM Θ and a sequence of observations $\mathbf{X} = \mathbf{x}_1, ..., \mathbf{x}_N$, find a plausible explanation, i.e. a sequence $\mathbf{Z}^* = \mathbf{z}^*_{1}, ..., \mathbf{z}^*_{N}$ of values of the hidden variable.

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Viterbi decoding

Z* is the overall most likely explanation of **X**:

$$\mathbf{Z}^* = \arg\max_{\mathbf{Z}} p(\mathbf{X}, \mathbf{Z} | \mathbf{\Theta})$$

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Posterior decoding

 \mathbf{z}_{n}^{*} is the most likely state to be in the *n*'th step: $\mathbf{z}_{n}^{*} = \arg \max_{\mathbf{z}_{n}} p(\mathbf{z}_{n} | \mathbf{x}_{1}, \dots, \mathbf{x}_{N})$

Summary

- Terminology of hidden Markov models (HMMs)
- Viterbi- and Posterior decoding for finding a plausible underlying explanation (sequence of hidden states) of a sequence of observation
- Next: Algorithms for computing the Viterbi and Posterior decodings efficiently