Hidden Markov models redux

ISTA 410 / INFO 510: Bayesian Modeling and Inference

U. of Arizona School of Information

April 28, 2021

Outline

Last time:

- Intro to hidden Markov models

Today:

- Review of HMM algorithms
- A pattern-recognition example

Note: office hours moved to Friday 1-3PM this week; Tuesday 1-3 PM next week.

Last HW / Data Diary

Last HW posted (HW 5)

- Bernoulli GLM with covarying slopes and intercepts
- Show that correlation between parameters can be a feature of the model rather than the data

Reflective assignment: statistics diary

- Create an empty text document
- Once a day for 7 days, add to your statistics diary
  - Entries can be anything; slice-of-life observations, research notes, etc.
  - Write as much or as little as you want
- Optional; can substitute for a missed HW

Temporal and dynamical models

Temporal and dynamical models

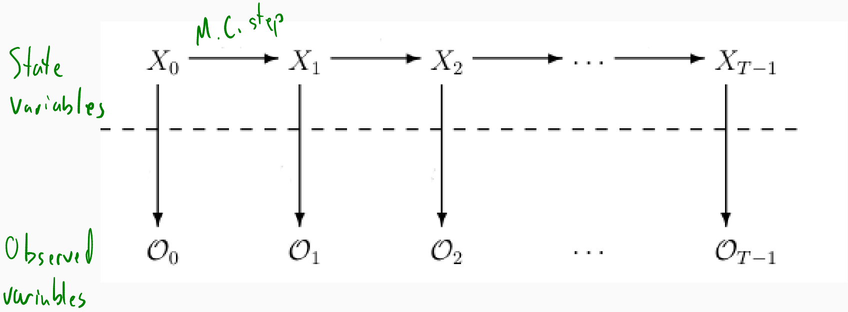
The models we'll look at next are used to model sequential data, especially time series.

- Hidden Markov model: latent state variables evolve according to a Markov chain/Markov process
- Linear dynamical system: latent state variables evolve according to linear dynamics, possibly with added noise

What these have in common: hidden/latent state variables

Hidden state models

Structure of the model:



- Latent/hidden system state
- Observations based on system state

Two state-observation models

Two common models:

- Hidden Markov model
  Hidden states evolve according to a Markov process
  Observations typically Gaussian or multinomial
- Linear Gaussian dynamical system
  States evolve according to linear dynamics
  Observations a linear function of the state, “corrupted” by Gaussian noise

Typical inference problems

Typical problems we want to solve, given a sequence of observations $\mathcal{O}$ of time length T:

- Filtering: find the distribution of X_T – that is, the distribution of the current state, accounting for all observations up to now.
- Prediction: find the distribution of X_t for some $t > T$.
- Smoothing: find the distribution of X_t for some $1 \leq t < T$. This looks very similar to filtering, but differs in that we can take the observations after time t into account.
- MAP or best-explanation: find the sequence (X_i) maximizing $P(\mathcal{O}, X)$.
- Fitting: Given a sequence of observations, estimate the parameters of the underlying dynamical model.

Hidden Markov models

Example: the unfair casino

A casino employee has two 6-sided dice. We'll assume we know their properties:

Die	$P(1)$	$P(2)$	$P(3)$	$P(4)$	$P(5)$	$P(6)$
fair	$1/6$	$1/6$	$1/6$	$1/6$	$1/6$	$1/6$
loaded	$1/2$	$1/10$	$1/10$	$1/10$	$1/10$	$1/10$

The operator throws a die, but you don't know which one. What is the probability the die is loaded, assuming it lands on 1? What if instead it lands on 3?

Tracking fairness over time

Let's say we know a little more about this casino employee's habits.

- The employee always starts the game with the fair die
- Every so often, they secretly switch the die
- Note: this is not an independent choice of die per throw

Result of this: streaks of fair/loaded die over time.

If we observe the result of the die rolls, can we infer when each die was in use?

Hidden Markov models

A hidden Markov model deals with two sequences:

- a sequence of *states*: the un-observed variable, changing over time according to a Markov chain model
- a sequence of *observations*, or *emissions*: the observed variable, with a distribution based on the current state

In our example:

- the state is which die is currently in use
- the emission is the roll of the die

Simplest case

In a HMM, the underlying states are governed by a Markov process.

Our simple example is a finite state, multinomial HMM:

- Underlying state X_t follows a Markov chain with N states
- Observed values $\mathcal{O}_t$ follow a multinomial distribution conditional on X_t

So the model is described by two matrices, A (transition matrix), and B (observation matrix).

$\pi = (1, 0)$

To do calculations, we also need to assume a certain distribution $\boxed{\pi}$ on the initial state X_1. As a shorthand, I'll use the notation $\lambda = (A, B, \pi)$ to represent a choice of these parameters.

Reference: Stamp, *A Revealing Introduction to Hidden Markov Models*

Simplest case

$\mathcal{O} = (\cdot, 1, 1)$

Assumptions:

$X = (\text{fair}, \text{loaded}, \text{loaded})$

- Initial state is always fair, so

$$\pi = (1, 0)$$

$P(X \cap \mathcal{O})$

$= \pi_{\text{fair}} \times 0.05 \times 0.5 \times 0.95 \times 0.5$

- Transition matrix:

$$A = \begin{pmatrix} 0.95 & 0.05 \\ 0.05 & 0.95 \end{pmatrix}$$

- Observation matrix:

$$B = \begin{pmatrix} 1/6 & 1/6 & 1/6 & 1/6 & 1/6 & 1/6 \\ 1/2 & 1/10 & 1/10 & 1/10 & 1/10 & 1/10 \end{pmatrix}$$

$\leftarrow$ dist for fair die

dist for loaded die.

Three algorithms

Today: standard algorithms for filtering, smoothing, and fitting:

1. Given a multinomial HMM λ and a sequence of observations $\mathcal{O}$, compute the distribution $P(X_t|\lambda, \mathcal{O})$.
2. Given a multinomial HMM λ and a sequence of observations $\mathcal{O}$, compute the probability distribution of X_t for some $1 \leq t \leq T$.
3. Given a sequence of observations $\mathcal{O}$, what is the multinomial HMM λ that maximizes the marginal likelihood $P(\mathcal{O}|\lambda)$?

Naïve filtering

It is clear that we can compute the joint probability of a particular sequence of states with the observed sequence:

$$P(\mathsf{X}, \mathcal{O}|\lambda) = \pi_{X_1} \prod_{t=1}^{T} A_{X_{t-1},X_t} B_{X_t,\mathcal{O}_t}$$

So, naïvely, we could compute this for all sequences of states, and then

$$P(X_t = x_i) = \sum_{\text{sequences with } X_t = x_i} P(\mathsf{X}, \mathcal{O}|\lambda)$$

What's the problem?

Naïve filtering

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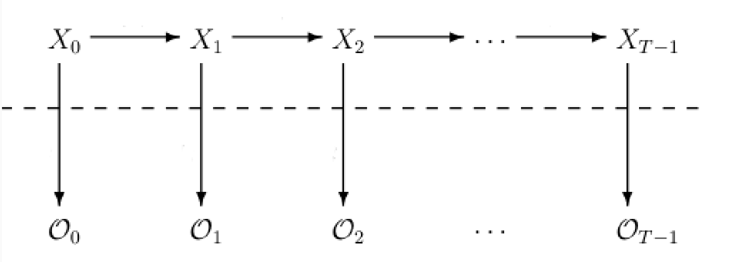
What's the problem? N^T sequences – computationally infeasible for all but short sequences.

The forward algorithm

This problem can be solved by the *forward algorithm*, which exploits the Markov property to marginalize recursively on the fly:



Let $\alpha_t(x_i) = P(X_t = X_i, \mathcal{O}|\lambda)$

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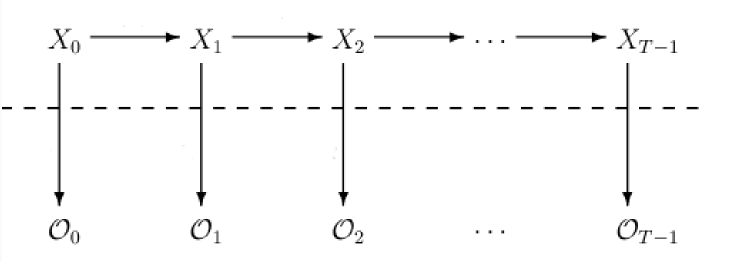

Let $\alpha_t(x_i) = P(X_t = X_i, \mathcal{O}|\lambda)$

$$\alpha_t(x_i) = B_{x_i,\mathcal{O}_i} \sum_{j=1}^{N} \alpha_{t-1}(x_j) A_{x_j,x_i}$$

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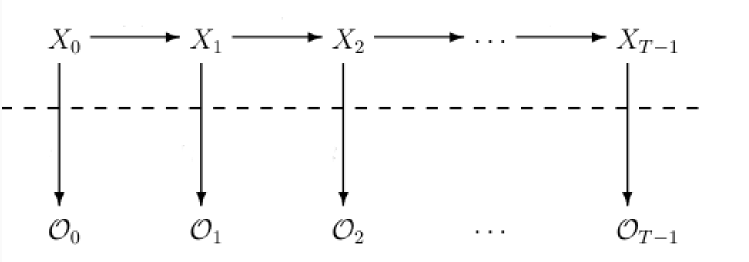


Let $\alpha_t(x_i) = P(X_t = X_i, \mathcal{O}|\lambda)$

$$\alpha_t(x_i) = B_{x_i,\mathcal{O}_i} \sum_{j=1}^{N} \alpha_{t-1}(x_j) A_{x_j,x_i}$$

Ex: assume $P(X_t = \text{fair}) = 0.8$

$P(X_t = \text{loaded}) = 0.2$

observe a 5 at time $t+1$

$$\underbrace{P(X_{t+1} = \text{fair} \cap \text{observe } 5)}_{\alpha_{t+1}(\text{fair})} = \overbrace{P(X_t = \text{fair})}^{\alpha_t(\text{fair})} \times P(\text{stayed fair}) \times P(5 \mid \text{fair})$$

$$+ \underbrace{P(X_t = \text{loaded})}_{\alpha_t(\text{loaded})} \times P(\text{switched}) \times P(5 \mid \text{fair})$$

$O(N^2)$ calculations to update $t \to t+1$; $N^2 T \ll N^T$

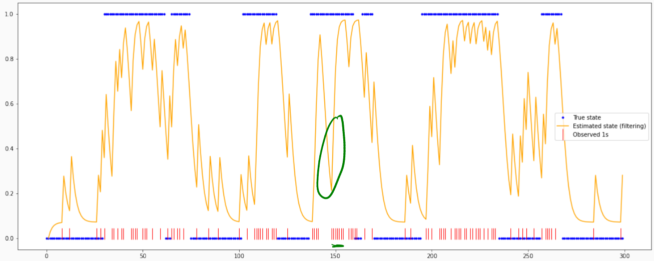
$$\alpha_T(i) = P(X_T = i \cap \theta)$$

$$P(X_T = i \mid \theta) = \frac{\alpha_T(i)}{\sum_j \alpha_t(j)}$$

Filtering result

To test, generate a sequence of states and observations, and run the forward algorithm:

loaded



fair

The backward pass

The smoothing problem asks us to calculate $P(X_t = x_i, \mathcal{O})$ for some $t < T$. We could just solve the filtering problem by running the forward algorithm up to time t, but we would lose the information from future states.

Solution: do a backward pass too.

Let $\beta_t(x_i) = P(\mathcal{O}_{t:T} | X_t = x_i)$; that is, the probability of the "remaining" observations from time t to the end, given $X_t = x_i$. Then,

$$\beta_t(x_i) = \sum_{j=1}^{N} A_{x_i,x_j} B_{x_i,\mathcal{O}_t} \beta_{t+1}(x_j)$$

so we can recursively calculate from the end of the sequence, letting $\beta_T(x_j) = 1$ for each j.

The forward-backward algorithm

The forward-backward algorithm solves the smoothing problem for HMMs:

$$P(X_t = x_i | \mathcal{O}, \lambda) = \frac{\alpha_t(x_i)\beta_t(x_i)}{P(\mathcal{O}|\lambda)}$$

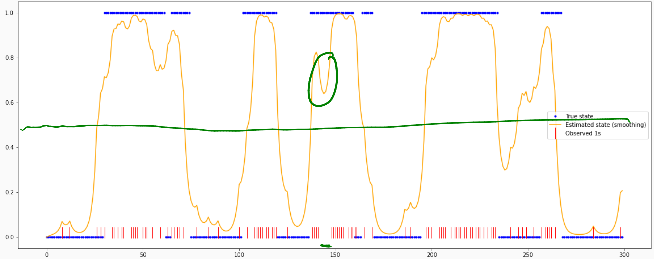
forward-backward alg for HMM very similar to CTC output layer for RNNs.

Where can we get the normalizing constant?

$$P(\mathcal{O}|\lambda) = \sum_{i=1}^{N} \alpha_T(x_i)$$

Smoothing result

To test, generate a sequence of states and observations, and run the forward-backward algorithm:



Aside: Viterbi algorithm

The forward-backward algorithm computes

$$P(X_t = i|\mathcal{O}, \lambda)$$

for each $1 \leq t \leq T$.

most probable state sequence/best explanation.

- Slightly different: MAP estimate of the state sequence
- Most probable sequence X may not equal the most probable state at each time step
- Viterbi algorithm (described in Stamp's article as *dynamic programming*) gives MAP estimate for the state sequence

Viterbi algorithm

Like the forward algorithm, the Viterbi algorithm exploits the Markov property to express the calculation recursively:

- Assume we can calculate the most probable sequences that end in states x_i at time $t-1$
- The most probable sequence that ends in state x_j at time t must be an extension of one of the N most probable sequences up to time $t-1$
- The most probable sequence overall must be the most probable sequence ending in state x_i at time T, for some i

$\mathcal{O}(N^2T)$

Viterbi algorithm

Essentially, we modify the forward algorithm to replace a sum with a max. Let:

$$\tilde{\alpha}_t(x_i) = P(X_{1:t} = \tilde{X}_{1:t,i}, \mathcal{O}_{1:t}|\lambda)$$

where $\tilde{X}_{1:t-1,i}$ is the most probable sequence of steps given $\mathcal{O}$ such that $X_t = x_i$.

$$\tilde{\alpha}_t(x_i) = \max_j \left(A_{x_j,x_i} B_{x_i,\mathcal{O}_t} \tilde{\alpha}_{t-1}(x_j)\right)$$

HMM fitting

Fitting parameters

The fitting problem gives a new challenge:

- Given a fixed state space $\{0, 1, \ldots, n\}$ and a sequence $\mathcal{O}$ of observations, find the model parameters that best fit the sequence $\mathcal{O}$
- i.e., tune A (transition matrix), B (observation matrix), and π (initial state distribution)
- Target: maximize $P(\mathcal{O}|A, B, \pi)$

This is a form of unsupervised learning.

Baum-Welch algorithm

(not named by stamp

The Baum-Welch algorithm iteratively improves the fit of the model parameters in a two-step process:

- Do a smoothing step, estimating the probability distributions of the hidden states X_t
- Re-adjust the model parameters to better fit this estimated distribution
- Score the model by the log-probability of the observed sequence
- Continue until log-probability change is negligible

End result: MAP estimate of model parameters

Idea behind BW algorithm

Intuitively:

- The smoothing step allows us to estimate the probability that the underlying chain is in each state x_i at time t
- We can use this to count the estimated probability of transitions from state x_i to state x_j
- We can use this, together with the observation sequence, to estimate the probability of each observation from state x_i

$\mathcal{O}(N^2 T)$

Estimating the transition matrix

Smoothing gives us:

$$\gamma_t(i) = \frac{\alpha_t(i)\beta_t(i)}{P(\mathcal{O}|A, B, \pi)}$$

which estimate the probability that the chain was in state x_i at time t. We extend this to:

"digamma"

$$\gamma_t(i,j) = \frac{\alpha_t(i) A_{ij} B_{j,\mathcal{O}_t}, \beta_{t+1}(j)}{P(\mathcal{O}|A, B, \pi)}$$

which estimates the probability that the chain was in state x_i at time t *and* state x_j at time $t+1$.

Then, we re-estimate the transition probability A_{ij} as:

$$A_{ij} = \frac{\sum_t \gamma_t(i,j)}{\sum_t \gamma_t(i)} \qquad T$$

Estimating the rest

Similarly, we can re-estimate the observation probability B_{ij} as

$$B_{ij} = \frac{\sum_{t,\mathcal{O}_t=j} \gamma_t(i)}{\sum_t \gamma_t(i)}$$

the expected proportion of the time spent in state i that produces observation j.

Estimating the rest

Similarly, we can re-estimate the observation probability B_{ij} as

$$B_{ij} = \frac{\sum_{t,\mathcal{O}_t=j} \gamma_t(i)}{\sum_t \gamma_t(i)}$$

the expected proportion of the time spent in state i that produces observation j.

The estimate of the initial state vector is just:

$$\pi_i = \gamma_0(i)$$

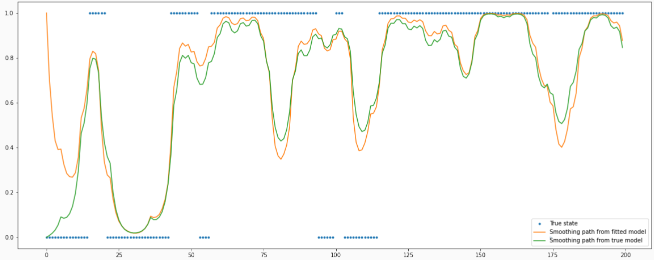
Testing the algorithm

Let's test the algorithm on the unfair casino problem:

- Generate 1200 observations from the "true" model
- Initialize a HMM with the correct number of states, but randomly initialized parameters
- Fit the model; test its performance on a smoothing problem

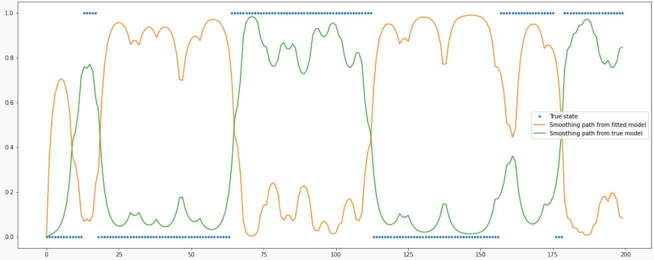
Testing the algorithm

Now: 200 new states and observations



Testing the algorithm

Another run of this experiment produced this:



Is this a failure of the fitting process?

Other applications

Because of their ability to find and recognize patterns in sequence data without supervision, HMMs find applications in, among other places:

- speech recognition
- cryptanalysis (codebreaking) and malware detection
- activity recognition
    - identify what an animal is doing based on GPS data

Text analysis example

Imagine you're an alien with no knowledge of human language, but you gain access to a sample of English text, and you would like to extract some information about the relationships between characters.

Simplifying assumptions:

- No cases – everything is lowercase
- No digits or punctuation; only characters are letters and spaces

Idea:

- different characters play different roles in the written language.
- fit a hidden Markov model with k different states to a large sample of text, and see if any patterns can be seen.

Let's take a look at the results for $k = 2$.

Expectation-maximization algorithms

EM algorithms

The Baum-Welch algorithm we saw before is an example of a much wider class of algorithms called *expectation-maximization* algorithms.

These are applicable when the observed data depends on hidden/latent state variables as well as model parameters. Roughly, the idea is:

- Expectation step: compute the distribution of hidden state variables, given current model parameters smoothing step
- Maximization step: compute the model parameters that maximize (log) likelihood given the state parameters from the expectation step update step.

Repeat until done – score model by total log-likelihood of the data.

Section 13.4-13.6 in BDA has another presentation of EM algorithms in a different context.

EM algorithms

Formally:

- θ: model parameters
- X: hidden variables
- Y: observations
- $L(\theta|X, Y)$: likelihood function

1. E-step: compute $Q(\theta|\hat{\theta}) = E_{X|Y,\hat{\theta}}[\log L(\theta|X, Y)]$
2. M-step: compute $\theta^{\text{new}} = \underbrace{\arg\max_{\theta} Q(\theta|\hat{\theta})}_{\text{maximum likelihood}}$

in the book

BW algorithm as EM

Recall the Baum-Welch algorithm has two steps:

- Perform smoothing to estimate the distribution of each X_t, given current transition/observation matrix values
- Update parameter values by counting transitions/observations given distributions of X_t

Although we don't explicitly calculate expectations of log-likelihoods, the smoothing step is an E step and the update step is an M step.

A few comments

Alternative approaches to parameter estimation

Other approaches to fitting HMM parameters:

- MCMC – suitable for smaller systems
  - Helmut Strey has a PyMC3 implementation
  - `https://github.com/hstrey/Hidden-Markov-Models-pymc3`
- Particle filter (aka sequential Monte Carlo) methods
  - Brief overview next Wednesday, time permitting

sampling based method

Gaussian HMM

The most common alternative to the multinomial distribution for HMMs is the Gaussian (normal) distribution. In this model:

- X_t still evolves according to a Markov chain with transition matrix A
- $\mathcal{O}_t \sim \mathrm{MVNormal}(\mu_{X_t}, \Sigma_{X_t})$
- Result: the observation distributions are Gaussian mixtures

Filtering and smoothing in Gaussian HMM

What has to change for our filtering and smoothing algorithms?

Filtering and smoothing in Gaussian HMM

What has to change for our filtering and smoothing algorithms?

- Only change: $P(\mathcal{O}_t = j | X_t = x_i)$ is no longer given by a matrix entry $\boxed{B_{ij}}$
- Instead, we have $p(\mathcal{O}_t = \mathrm{y} | X_t = x_i) = \overbrace{\mathrm{MVNormal}(\mu_i, \Sigma_i)}^{\text{mvnorm pdf}}$ for a certain mean vector μ_i, covariance matrix Σ

EM for Gaussian HMM

To fit the Gaussian HMM, we only need to make the following modifications to the M step:

- Replace B_{ij} with $\boldsymbol{\mu}_i, \Sigma_i$
- Replace the update of B_{ij} with a maximum-likelihood estimate for a Gaussian, weighted by the estimated state probabilities (from smoothing):

$$\boldsymbol{\mu}_i^{\text{new}} = \frac{\sum_t P(X_t = i)\boldsymbol{y}_t}{\sum_t P(X_t = i)}$$

$$\Sigma_i^{\text{new}} = \frac{\sum_t P(X_t = i)(\boldsymbol{y}_t - \boldsymbol{\mu}_i^{\text{new}})(\boldsymbol{y}_t - \boldsymbol{\mu}_i^{\text{new}})^T}{\sum_t P(X_t = i)}$$

where y_i are the observations.

Missing data

Suppose we have an incomplete sequence of observations:

$$(\mathcal{O}_t) = (\mathcal{O}_1, \mathcal{O}_2, \ldots, \mathcal{O}_T)$$

where some $\mathcal{O}_t$ are unobserved (NA).

We can still perform forward and backward algorithms for filtering/smoothing; however, steps where $\mathcal{O}_t = NA$ only involve transition probabilities, no observation.

Result: estimated distribution of hidden states relaxes toward the stationary distribution of the MC during "gaps" in observations

Continuous time

Continuous-time Markov chains do exist, so we could build a HMM on top of one of those.

- Applications:
- How a CT-MC works:
  - Each state x_i has an associated *holding time* – an exponential random variable
  - Chain stays in current state for the holding time and then undergoes a transition according to a transition matrix
- Challenge: transition times are unobserved, and may not correspond to the observation times

Continuous time

Reduction to discrete HMM:

- The continuous time chain can be expressed in terms of a *transition rate matrix* Q
- Each entry q_{ij} gives the rate parameter for an exponential random variable; transitions from state i are determined by the minimum of the exponential random variables
- Can reduce to a discrete-time Markov chain with transition matrix dependent on the time interval between two observations: $P(t) = \exp(Qt)$

Details: Liu et al., "Efficient Learning of Continuous-Time Hidden Markov Models for Disease Progression" (2015)

Summary

Today:

- Applications of hidden Markov model fitting

Next week:

- Linear Gaussian dynamical systems and the Kalman filter
- Forward filtering/backward sampling algorithms
- Particle filter algorithms (maybe?)