Dynamic and temporal models

ISTA 410 / INFO 510: Bayesian Modeling and Inference

U. of Arizona School of Information

April 26, 2021

Outline

Last time:

- Gaussian process regression

Today:

- Overview of temporal models
- Intro to hidden Markov models

Aside: HW example

Reed frog example from HW

Recall the reed frog example from HW4:

- 48 tanks of reed frog tadpoles
    - Different numbers of tadpoles per tank
    - Large and small tanks
    - Some tanks exposed to predators

binary categorical

- Problem: estimate survival rates, effect of predation and tank size

Reed frog example from HW

2 models on HW, 1 not:

- Fully pooled model: pool together all tanks with/without predators and estimate parameters for

$$y_i \sim \text{Binomial}(n_i, p_i)$$
$$\text{logit}(p_i) = \alpha + \beta_p \text{pred}$$

Alternate parameterization

α_{pred} ← each tank with pred observes this

α_{nopred} ← each tank w/o pred observes this.

- Unpooled model: each tank gets its own estimate of the intercept for

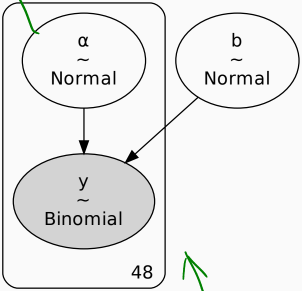
$$\text{logit}(p_i) = \alpha_i + \beta_p \text{pred}$$

Each tank has its own α, adjust for predation.

- Partially pooled: each tank gets its own estimate of the intercept, but the prior parameters for the intercept are pooled

Plate diagrams

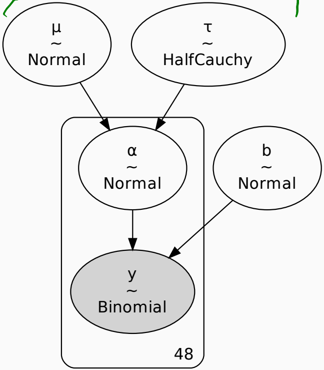
all alphas come independently from $N(0,2)$



48 intercepts + 1 slope to estimate 48 survival rates

unpooled

scale of random variation between tanks is learned / estimated from data



partially pooled

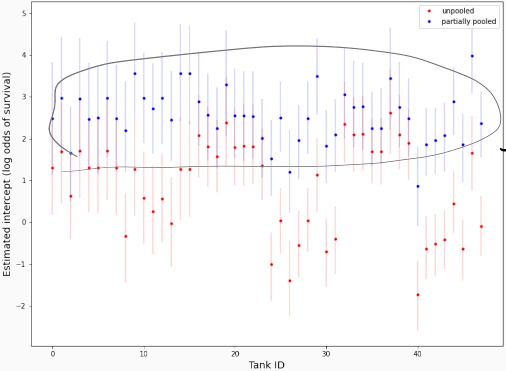
Results

Interesting feature: estimated predation effect

- Unpooled model: estimates zero predation effect
- Partially pooled model: strong predation effect
    - Intuition and data inspection tells us the unpooled model must be wrong
    - Problem: both models are over-parameterized, so need some regularization/prior knowledge

Results

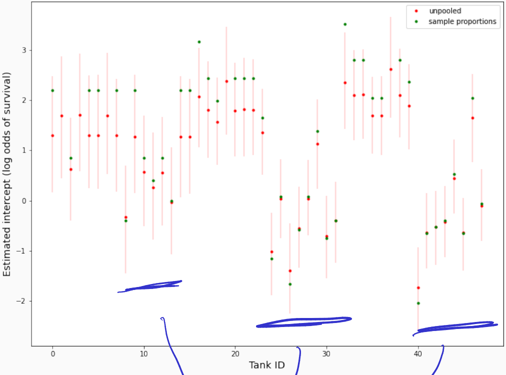
Estimated intercepts from the two models:



intercepts all in an interval of width ≈ 2 on log-odds scale

Results

Estimated unpooled intercepts, with sample proportions:



predation

Interpretation

- The unpooled model has too much freedom to account for differences between tanks in the intercept
- Differences that are due to predation are folded into the random between-tank variation
- Partially-pooled model doesn't allow individual intercepts to stray too far from one another
    - Difference due to predation too large to fit into the between-tank variation
    - Predation effect estimated instead

Temporal and dynamical models

Temporal and dynamical models

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

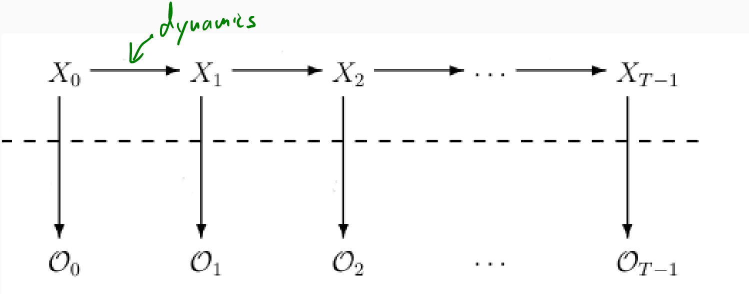
- Hidden Markov model: latent state variables evolve according to a Markov chain/Markov process
- Linear dynamical system: latent state variables evolve according to linear dynamics, possibly with added noise

What these have in common: hidden/latent state variables

Hidden state models

We're going to focus on hidden state models, which have a general structure similar to below:

Hidden states



Observed variables

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

Two state-observation models

Two common models:

finite-state
each state is multinomial,
dependent only on previous state.

- 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?

Bayes: If you see a 1 : $P(\text{loaded}) = 3/4$

If you see anything else : $P(\text{loaded}) = 3/8$

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).

To do calculations, we also need to assume a certain distribution π 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*

Three algorithms

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

filtering 1. Given a multinomial HMM λ and a sequence of observations $\mathcal{O}$, compute the distribution $P(X_t|\lambda, \mathcal{O})$.

smoothing 2. Given a multinomial HMM λ and a sequence of observations $\mathcal{O}$, compute the probability distribution of X_t for some $1 \leq t \leq T$.

fitting 3. Given a sequence of observations $\mathcal{O}$, what is the multinomial HMM λ that maximizes the marginal likelihood $P(\mathcal{O}|\lambda)$?

estimate properties of dice
estimate how often dice are switched.

Naïve filtering

$\Pi = (\Pi_1, \Pi_2, \dots)$ $\pi = (1, 0)$

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

$$P(X, \mathcal{O}|\lambda) = \underbrace{\overbrace{\pi_{X_1}}^{\text{initial state}} \prod_{t=1}^{T} \overbrace{A_{X_{t-1},X_t}}^{\text{transition matrix}}}_{P(X)} \underbrace{\overbrace{B_{X_t,\mathcal{O}_t}}^{\text{observation matrix}}}_{P(\mathcal{O}|X)}$$

Hypothetical:
fair, fair, loaded, fair, fair, ...

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

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

What's the problem?

Naïve filtering

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

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

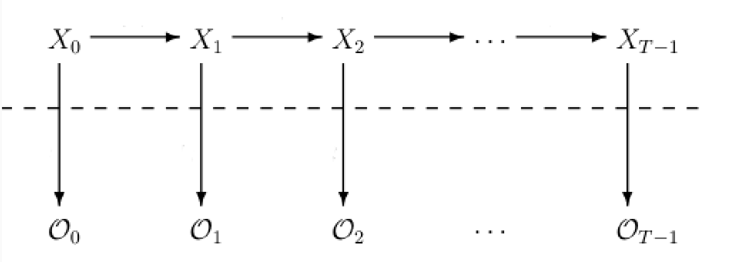
So, naïvely, we could compute this for all sequences of states, and then

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

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

N = # of states ; T = # of time steps

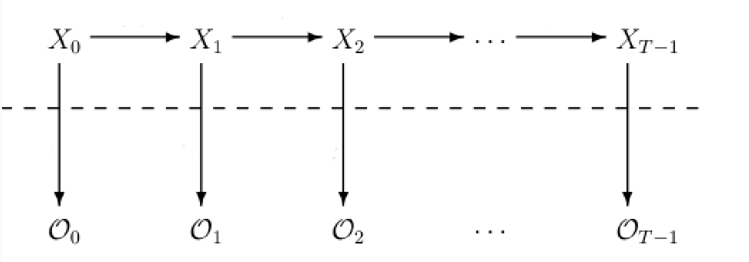
This problem can be solved by the *forward algorithm*, which exploits the Markov property to marginalize recursively on the fly:



Let $\alpha_t(x_i) = P(X_t = \overset{i}{\cancel{x_i}}, \mathcal{O}|\lambda)$ = prob that chain is in state i at time t, joint with observed sequence.

The forward algorithm

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



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

P(state i at time t)

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

= P(state j at time t-1)

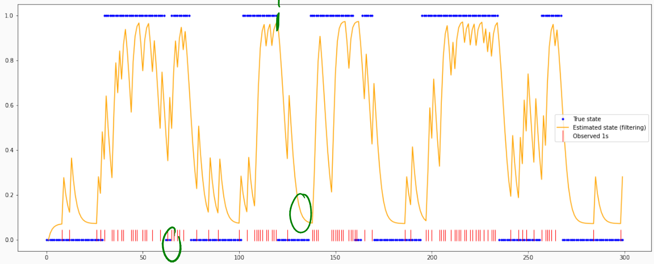
$\times A_{j \to i} \times B_{i \to \mathcal{O}_t}$

sum over j

Filtering result

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

$t \approx 110$



not enough data to detect this

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

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:

$$P(X_t = x_i|\mathcal{O},\lambda) = \frac{\overbrace{\alpha_t(x_i)}^{\text{information from 0 to t}}\overbrace{\beta_t(x_i)}^{\text{info. from t to T}}}{P(\mathcal{O}|\lambda)}$$

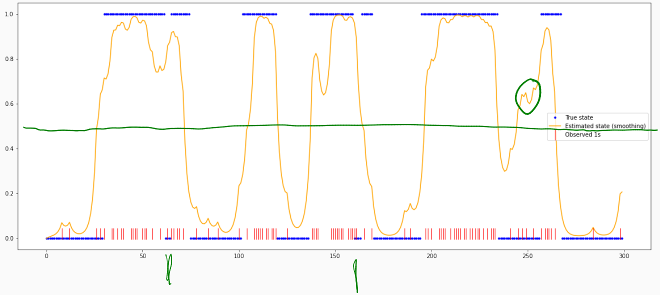
normalizing const.

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:



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 $\underline{P(\mathcal{O}|A, B, \pi)}$

This is a form of unsupervised learning.

Baum-Welch algorithm

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

prediction
- Do a smoothing step, estimating the probability distributions of the hidden states X_t

update
- 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

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:

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

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:

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

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:

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

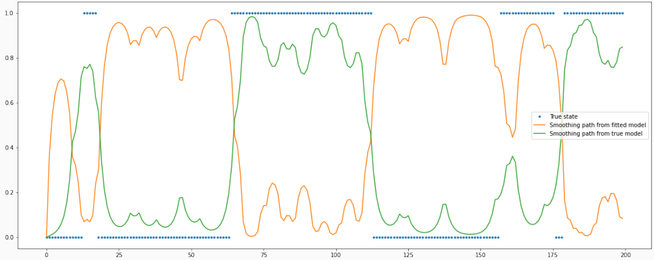
Testing the algorithm

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

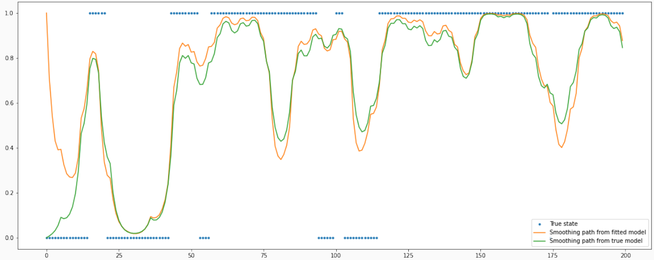
Testing the algorithm

Now: 200 new states and observations



Testing the algorithm

Another run of this experiment produced this:



~~Is this a failure of the fitting process?~~

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
- Maximization step: compute the model parameters that maximize (log) likelihood given the state parameters from the expectation 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 $\theta^{\text{new}} = \arg\max_{\theta} Q(\theta|\hat{\theta})$

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.

Summary

Today:

- Intro to hidden Markov models

Going forward:

- Estimating HMM parameters; E-M algorithms; modern MCMC and other estimation for HMMs
- Other HMM applications
- Linear Gaussian dynamical systems and the Kalman filter

A few comments

Gaussian HMM

The most common alternative 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 B_{ij}
- Instead, we have $p(\mathcal{O}_t = \mathrm{y} | X_t = x_i) = \mathrm{MVNormal}(\mu_i, \Sigma_i)$ 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

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
- 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)