HMMs for Complex Biologging Data

CANSSI Collaborative Research Team Project #22

Day 2

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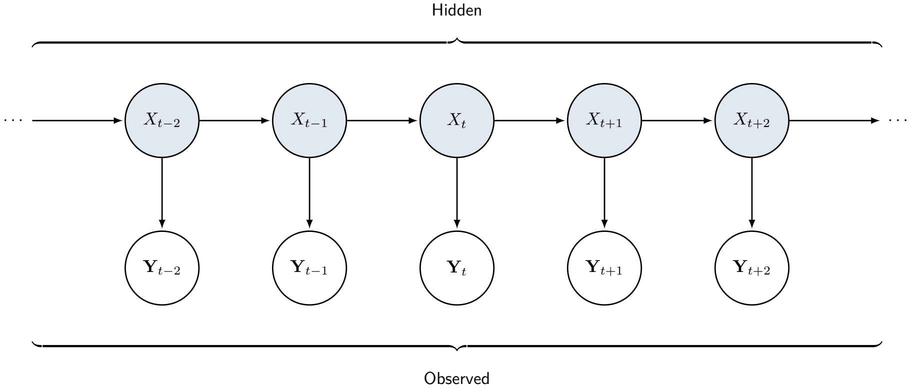
Day 1 Recap

- Finite mixture models
- Markov chains
- Hidden Markov models
- Forward and backward variables
- Likelihood computations

Day 1 Recap


Hidden
$\cdots$
X_{t-2}
X_{t-1}
X_t
X_{t+1}
X_{t+2}
$\cdots$
$\mathbf{Y}_{t-2}$
$\mathbf{Y}_{t-1}$
$\mathbf{Y}_t$
$\mathbf{Y}_{t+1}$
$\mathbf{Y}_{t+2}$
Observed

Decoding

- Once the parameters $\boldsymbol{\eta}$ of the model have been estimated, we can do several things with the estimates

- While the estimates provide information about the data-generating process, they can also help us determine the states $x_{1:T}$ which were most likely to give rise to the observed data $Y_{1:T}$

- Classifying (or *decoding*) the unknown state sequence $X_{1:T}$ can be accomplished using several algorithms

Local and Global Decoding

- *Local decoding* refers to the classification of each X_t individually by setting

$$\hat{X}_t = \underset{x \in \mathcal{X}}{\text{argmax}} \, \mathbb{P}_{\hat{\boldsymbol{\eta}}} \left(X_t = x \mid Y_{1:T} = y_{1:T} \right), \quad t = 1, \ldots, T$$

- In words, we choose the state that maximizes the *a posteriori* state membership probability

- In contrast, *global decoding* classifies the entire state sequence at once:

$$\widehat{X_{1:T}} = \underset{x_{1:T} \in \mathcal{X}^T}{\text{argmax}} \, \mathbb{P}_{\hat{\boldsymbol{\eta}}} \left(X_{1:T} = x_{1:T} \mid Y_{1:T} = y_{1:T} \right)$$

- Here, we focus on local decoding (in practice, both methods tend to produce similar classifications)

Interlude: Backward Variables

- Yesterday, we introduced the *forward variables* $\alpha_{x,t} = f_{\hat{\boldsymbol{\eta}}}\left(Y_{1:t} = y_{1:t}, X_t = x\right)$

- Now, we will also need the *backward variables* $\beta_{x,t} = f_{\hat{\boldsymbol{\eta}}}\left(Y_{(t+1):T} = y_{(t+1):T} \mid X_t = x\right)$

- As with the forward variables, the vectors of backward variables $\boldsymbol{\beta}_t = (\beta_{1,t}, \ldots, \beta_{K,t})^\top$ can be computed recursively in polynomial time via dynamic programming

- In particular, if

$$\mathbf{P}(y) = \begin{pmatrix} f_1(y) & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & f_K(y) \end{pmatrix},$$

  then it is easily shown that $\boldsymbol{\beta}_t = \boldsymbol{\Gamma}\mathbf{P}(y_{t+1})\boldsymbol{\beta}_{t+1}$ for $t = 1, 2, \ldots, T-1$

Local Decoding

- Local decoding is accomplished using forward variables

$$\alpha_{x,t} = f_{\hat{\boldsymbol{\eta}}}\left(Y_{1:t} = y_{1:t},\, X_t = x\right)$$

and backward variables

$$\beta_{x,t} = f_{\hat{\boldsymbol{\eta}}}\left(Y_{(t+1):T} = y_{(t+1):T} \mid X_t = x\right)$$

- Since

$$\alpha_{x,t} \cdot \beta_{x,t} = f_{\hat{\boldsymbol{\eta}}}\left(Y_{1:T} = y_{1:T},\, X_t = x\right),$$

Bayes' rule yields

$$\mathbb{P}_{\hat{\boldsymbol{\eta}}}\left(X_t = x \mid Y_{1:T} = y_{1:T}\right) = \frac{f_{\hat{\boldsymbol{\eta}}}\left(Y_{1:T} = y_{1:T},\, X_t = x\right)}{f_{\hat{\boldsymbol{\eta}}}\left(Y_{1:T} = y_{1:T}\right)} = \frac{\alpha_{x,t} \cdot \beta_{x,t}}{L_T}$$

Local Decoding

- Local decoding thus sets

$$\hat{X}_t = \underset{x \in \mathcal{X}}{\text{argmax}} \left(\frac{\alpha_{x,t} \cdot \beta_{x,t}}{L_T} \right) = \underset{x \in \mathcal{X}}{\text{argmax}} \left(\alpha_{x,t} \cdot \beta_{x,t} \right), \quad t = 1, \ldots, T$$

- The computation of these conditional probabilities via forward and backward variables is known as the *forward-backward algorithm*

Covariates in State Dependent Distributions

- The basic HMM may be too simplistic a model for certain applications
- Occasionally, we might want certain parameters in the model to depend on covariates (for example, an animal's sex, weight, age, etc.)
- For example, the state-dependent mean θ_x might depend linearly on some fixed vector $\mathbf{z} \in \mathbb{R}^p$, perhaps through some link function g :

  $$g(\theta_x) = g\left(\mathbb{E}\left[Y_t \mid X_t = x\right]\right) = \boldsymbol{\beta}_x^\top \mathbf{z},$$

  where $\boldsymbol{\beta}_x^\top = (\beta_{x,1}, \ldots, \beta_{x,p})$ is a vector of regression coefficients
- In other words, each state-dependent distribution carries its own generalized linear model

Covariates in Transition Probabilities

- Alternatively, we may incorporate covariates into each of the $K \cdot (K-1)$ transition probabilities

- This is typically accomplished by applying a multinomial logistic regression model to each row of the transition matrix:

$$\gamma_{j,x} = \mathbb{P}_{\boldsymbol{\eta}}\left(X_t = x \mid X_{t-1} = j\right) = \frac{e^{\boldsymbol{\beta}_{x|j}^{\top}\mathbf{z}}}{1 + \sum_{k=1}^{K-1} e^{\boldsymbol{\beta}_{k|j}^{\top}\mathbf{z}}}, \quad x, j \in \mathcal{X}$$

with $\boldsymbol{\beta}_{K|j} = \mathbf{0}$ for all $j \in \mathcal{X}$

More on Covariates

- In either case, the $\boldsymbol{\beta}_x$'s and/or $\boldsymbol{\beta}_{x|j}$'s are incorporated into the likelihood function and inference proceeds as usual
- We might also want to include covariates $\mathbf{z}_t$ that depend on time (for example, $\mathbf{z}_t$ could include the number of hours an animal has been awake at time t)
- In this case, inference proceeds in a similar fashion; however...
- Including time-varying covariates in the transition probabilities $\gamma_{j,x}$ destroys the assumption of time homogeneity, so each of the initial probabilities $\pi_x = \mathbb{P}_{\boldsymbol{\eta}}\left(X_1 = x\right)$ must also be estimated

Mixed HMMs

- We may have *multiple* time series — say S of them — available for inference
- When the time series are believed to be iid, they can be pooled together in a straightforward manner
- More realistically, the S time series are not iid, but still arise from HMMs with common features (such as the same underlying set of states $\mathcal{X}$)
- When the time series arise from the same parametric model (but with series-specific parameters), there can be up to $S \cdot \text{length}(\boldsymbol{\eta})$ parameters to estimate, which is cumbersome
- For example, there would be S state-dependent parameters for state j: $\theta_{j,1}, \ldots, \theta_{j,S}$

Random Effects

- Instead, one could regard the $\theta_{j,s}$'s as continuous random variables: $\theta_{j,1}, \ldots, \theta_{j,S} \overset{iid}{\sim} g_{\boldsymbol{\sigma}_j}$
- That is, each $\theta_{j,s}$ is a *random effect* with distribution $g_{\boldsymbol{\sigma}_j}$
- Each inclusion of such a random effect in the model reduces the number of parameters to estimate by $S - \text{length}(\boldsymbol{\sigma}_j)$
- The drawback, however, is that the $\theta_{j,s}$ must be integrated out of the likelihood:

$$\mathcal{L}(\ldots, \boldsymbol{\sigma}_j) = \int \cdots \int \mathcal{L}(\ldots, \theta_{j,1}, \ldots, \theta_{j,S}) \prod_{s=1}^{S} \left(g_{\boldsymbol{\sigma}_j}(\theta_{j,s}) \, \mathrm{d}\theta_{j,s} \right)$$

Discrete Random Effects

- Even for the simplest distributions $g_{\boldsymbol{\sigma}_j}$, such integrals are never available in closed form and must be computed numerically (which is difficult in high dimensions)

- Alternatively, one can assume the $\theta_{j,s}$'s to be *discrete* random variables on a finite sample space $\mathcal{M}$

- This makes for a much simpler likelihood computation:

$$\mathcal{L}(\ldots,\boldsymbol{\sigma}_j) = \sum_{s=1}^{S} \sum_{m\in\mathcal{M}} \mathcal{L}(\boldsymbol{\eta},\theta_{j,1},\ldots,\theta_{j,S}) \cdot \mathbb{P}_{\boldsymbol{\sigma}_j}\left(\theta_{j,s}=m\right)$$

- However, the applicability of such models may be limited

- The same ideas can be extended to dependent random effects, in which two or more parameters in the model follow a joint distribution

Multivariate Observations

- Until now we have assumed that each Y_t is a random variable
- However, everything discussed so far applies verbatim if the observations are d-dimensional *random vectors* $\mathbf{Y}_t = (Y_{t,1}, \ldots, Y_{t,d})$
- An often-used simplifying assumption is that of *contemporaneous conditional independence*:

$$\mathbf{Y}_t \mid (X_t = x) \sim f_x(\mathbf{y}) = \prod_{h=1}^{d} f_{x,h}(y_h)$$

- In other words, the components of $\mathbf{Y}_t$ are assumed to be independent

Multivariate Observations

- The assumption of contemporaneous conditional independence makes inference almost as easy as that for univariate HMMs
- However, it is sometimes too strong (for example, occupancy)
- In such cases, one can choose a non-factorial multivariate distribution to better model the dependence between the components of $\mathbf{Y}_t$
- The drawback is that for most such distributions, inference can be challenging
- Parameter estimates are available in closed form for the multivariate normal distribution, but little else
- One can use copulas to model arbitrarily complex dependence structures, although parameter estimation then requires new techniques [Zimmerman et al., 2022]

Bayesian Inference

- One can also perform Bayesian inference on HMMs
- To do so, one must choose an appropriate prior distribution $\pi(\boldsymbol{\eta})$ for the unknown parameters of the model
- The rows of the transition matrix $\boldsymbol{\Gamma}_k$ and the initial distribution $\boldsymbol{\pi}$ are traditionally assigned Dirichlet priors (which are conjugate to the multinomial distribution)
- Priors for the parameters θ_x of the state-dependent distributions are chosen on a case-by-case basis

Bayesian Inference

- The posterior distribution

$$\pi(\boldsymbol{\eta} \mid y_{1:T}) \propto \pi(\boldsymbol{\eta}) \cdot \mathcal{L}(\boldsymbol{\eta})$$

  is never available in closed form and is impossible to sample from directly

- Thus, Markov chain Monte Carlo (MCMC) methods are typically required to sample from it

- A popular choice of MCMC method for HMMs is Hamiltonian Monte Carlo (or variants thereof), as implemented in the Stan programming language

- Although written in C++, Stan has an R interface which is accessed through the `rstan` library

Quantifying Uncertainty

- As in all statistical inference, it is always of interest to quantify uncertainty in estimates of unknown parameters
- For frequentist inference, asymptotic normality of the MLE has been proven under mild regularity conditions [Bickel et al., 1998]
- The observed information matrix — which itself is a consistent estimator of the Fisher information — can be approximated numerically, and this yields standard errors and confidence intervals for parameter estimates
- In the Bayesian setup, credible intervals can be obtained from posterior distributions using standard techniques

Thank you!

References

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