Recap HSMM
Why considering random effects in H(S)MM?
General model of an H(S)MM with mixed effects
Overview of articles
Article details
Conclusion
References

# Review of estimation algorithms of HMM/HSMM with mixed effects

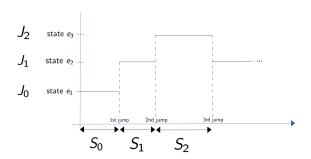
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# Recap HSMM (explicit duration)

 $S_n =$  **dwell time** of the *n*-jump  $J_n =$  the **n**-state visited



**Markov chain** :  $P(S_n|J_n = k) = \text{Geometric } (p_k)$ 

**Semi-Markov chain** (explicit duration) :  $P(S_n|J_n = k) =$ any law, Poisson  $(\lambda_k) + 1$  for example

## Variability impact of a qualitative covariate (as in GLMM)

Qualitative covariate's effects can be traited as random, when we are not particularly interested in the effect of each modality, but rather in the law of the effects.

Taking account long-range dependency (in HMM) [2] The observed variables  $(Y_t)_t$  are already not independent without random effects, but

$$Cov(Y_t, Y_{t+h}) \xrightarrow[h \to +\infty]{} 0$$

And with random effects in the model, under some (restrictive) conditions

$$Cov(Y_t, Y_{t+h}) \xrightarrow[h \to +\infty]{} k > 0$$

Notation : U = vector of all random effects.

For individual/trajectory number i,  $Y^i =$ **observed process**,  $Z^i =$ **hidden process**.

#### Definition

- *U* is a centred Gaussian vector (most of the time)
- Given U = u and the covariates,
  - $\{(Y^i, Z^i)\}_{1 \le i \le \mathcal{I}}$  are mutually independent
  - $\bullet$   $(Y^i, Z^i)$  is an **H(S)MM** impacted by u and the covariates of individual number i
  - Every law that compose the H(S)MM (for explicit duration case) :
    - emissions laws
    - transitions laws
    - dwell time laws
    - initial state law

belong to the exponential family, and the expected value depends linearly on u and covariates through a link function.

#### **Example of HMM**, with random effect specific to individual and state

- Emissions laws:

$$f(y_t^i|Z_t^i = k, U = u) = \exp\left(\frac{y_t^i \eta_{k,u}^i - b(\eta_{k,u}^i)}{\phi_k} - c(y_t^i, \phi_k)\right)$$
$$\eta_{k,u}^i = x^{i'} \beta_k^{(1)} + u_k^{i,(1)} \qquad \text{with } u_k^{i,(1)} \sim \mathcal{N}(0, \sigma_k^2)$$

 $\longrightarrow$  In each state k, we have a different GLMM regression.

- Hidden process laws:

$$P(Z_{t+1}^{i} = \mathbf{I}|Z_{t}^{i} = \mathbf{k}, U = u) = \frac{\exp\left(x^{i'}\beta_{\mathbf{k},\mathbf{l}}^{(2)} + u_{\mathbf{k},\mathbf{l}}^{i,(2)}\right)}{1 + \sum_{\alpha} x^{i'}\beta_{\mathbf{k},\alpha}^{(2)} + u_{\mathbf{k},\alpha}^{i,(2)}}$$

with 
$$u_{k,l}^{i,(2)} \sim \mathcal{N}(0, \sigma_{k,l,(2)}^2)$$

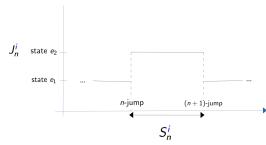
 $\longrightarrow$  In each state k, we have a different GLMM (multinomial) regression.

Each article is modelled as a special case, or with a design vector for random effects, or with dynamical covariates.

5/16

**Example of HSMM**, for dwell time only with random effect specific to individual and state

For the individual/trajectory number i:  $S_n^i =$ **dwell time** of the n-jump of the hidden process  $J_n^i =$ the n-state visited by the hidden process.



- dwell time, modelled by a Poisson:

$$\begin{split} P(S_n^i|J_n^i = \mathbf{k}, U = u) &= \mathcal{P}(\lambda_{\mathbf{k},u}^i) + 1 \\ \lambda_{\mathbf{k},u}^i &= \exp\left(x^{i\prime}\beta_{\mathbf{k}} + u_{\mathbf{k}}^i\right) & \text{with } u_{\mathbf{k}}^i \sim \mathcal{N}(0,\sigma_{\mathbf{k}}^2) \end{split}$$

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#### **Estimation problems**

- The integration over random effects is intractable.
- Fixed effects also introduce maximisation difficulties. These are problems derived from GLMM.

Several estimation methods are available.

EM	Newton-Raphson on the likelihood	Likelihood approximation, and maximisation	Bayesian
- Altman (2007) Monte-Carlo EM (MCEM) HMM - Chaubert (2008) Restoration- Maximisation, with Monte-Carlo HSMM - Maruotti (2011) no detail HMM - Delattre, Lavielle (2012) Stochastique Approximation EM (SAEM) (Monte-Carlo)	Haji-Maghsoudi & al. (2021) Monte-Carlo Newton- Raphson HSMM	- Altman (2007) Gaussian quadrature HMM  - Altman (2007) Importance sampling HMM  - Michelot (2023) Laplace quadrature HMM  - Koslik (2024) Laplace quadrature with quasi-REML in addition (integration over fixed effects of the likelihood) HMM	- Michelot (2023) MCMC Hamiltonian HMM

Notation : Y = all observed process, Z = all hidden process, U = all random effects,  $f^{\theta} =$  density function.

#### **EM**

#### step E

$$\begin{split} Q(\theta|\theta^{(m)}) &= E_{\theta^{(m)}} \left[ \log f^{\theta}(y, \mathbf{Z}, U) | Y = y \right] \\ &= E_{\theta^{(m)}} \left[ \underbrace{E_{\theta^{(m)}} \left[ \log f^{\theta}(y, \mathbf{Z}|U) | U, Y = y \right]}_{=:h_{\theta^{(m)}}(\theta, U, y)} | Y = y \right] + E_{\theta^{(m)}} \left[ \log f^{\theta}(U) | Y = y \right] \end{split}$$

Integration over Z is possible : the function  $h_{\theta^{(m)}}(\theta, u, y)$  can be calculated analytically by forward-backward for a given u.

 $\longrightarrow$  Need to approximate integration over U.

#### step M

Maximisation by Newton-Raphson (or quasi-Newton) most of the time

EM	Altman (2007)	Chaubert (2008) HSMM	Maruotti (2011) HMM	Delattre, Lavielle (2012)
random effetcs on <b>observed</b> process	V	V (gaussian em- mision only)	V	V
random effetcs on <b>hidden</b> pro- cess	V	X	X	V
Dynamical co- variates	V	X	V	X
E step	Monte-Carlo EM (MCEM)	Restoration- Maximisation, with Monte- Carlo at times	- Gaussian ran- dom effects: no details - Finite random effects: leads to special mix- ture of HMM.	Stochastic Approximation EM (SAEM) (Monte-Carlo). Convex combination between $\hat{Q}(. \theta^{(m-1)})$ and new simulation under $\theta^{(m)}$
M step	quasi-Newton	closed form (be- cause gaussian emissions)	no details	no details

Notation : Y = all observed process, Z = all hidden process, U = all random effects,  $f^{\theta} =$  density function.

#### **Newton-Rahpson**

$$abla_{ heta} \log f^{ heta}(y) = E_{ heta} \left( \ 
abla_{ heta} \log f^{ heta}(y, \mathbf{Z}, \mathbf{U}) \ | \mathbf{Y} = \mathbf{y} 
ight)$$

$$\nabla^2_{\theta} \mathsf{log} f^{\theta}(y) = E_{\theta} \left( \ \nabla^2_{\theta} \mathsf{log} f^{\theta}(y, \textbf{\textit{Z}}, \textbf{\textit{U}}) \ | \textbf{\textit{Y}} = \textbf{\textit{y}} \right) + \mathsf{Var}_{\theta} \left( \ \nabla_{\theta} \mathsf{log} f^{\theta}(y, \textbf{\textit{Z}}, \textbf{\textit{U}}) \ | \textbf{\textit{Y}} = \textbf{\textit{y}} \right)$$

Like EM, integration over Z is analytically possible with forward-backward, with the exception of the variance term in the Hessian (in fact I don't know)

 $\longrightarrow$  Need to approximate integration over U.

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EM Newton-Raphson on the likelihood Likelihood approximation, and maximisation

#### **Newton-Rahpson**

Haji-Maghsoudi & al. (2021) Monte-Carlo Newton-Raphson HSMM, random effects on <u>observed</u> process. Notation : Y = all observed process, Z = all hidden process, U = all random effects,  $f^{\theta} =$  density function.

### Likelihood approximation, and maximisation

$$L( heta,y)$$
 is an approximation of the likehood  $f^ heta(y)=\int f^ heta(y,u)\mathsf{d} u$ 

$$\hat{\theta} = \operatorname*{argmax}_{\theta} L(\theta, y)$$

$$f^{\theta}(y, u) = f^{\theta}(y|u)f^{\theta}(u)$$
 with  $f^{\theta}(y|u)$  calculable by forward.

Maximisation Newton-Raphson (or quasi-Newton) most of the time.

#### Likelihood approximation, and maximisation

	<b>Altman</b> (2007)	<b>Altman</b> (2007)	Michelot (2023)	Koslik (2024)
	HMM	HMM	HMM	HMM
random effetcs on observed process	V	V	V	V
random effetcs on hidden pro- cess	V	V	V	V
Dynamical covariates	V	V	V	V
Approximation'	s Gaussian quadra-	Importance	Laplace quadra-	Laplace quadra-
type	ture + quasi-Newton	sampling on $\int f^{\theta}(y,u) du + quasi-Newton$	ture on $\int f^{\theta}(y,u) du + package$ optimix for maximisation	ture on $\int f^{\theta}(y, u) du d\beta$ (with $\theta = (\beta, \sigma^{2}),$ $\beta = \text{fixed effects})$

#### Things to remember

- HSMMs are not frequently consider
- EM and likelihood approximation well represented, unlike Newton-Raphson and Bayesian
- No realy comparison between methods, except :
  - few random effects per individual => small integration dimension : quadrature are efficient (faster than Monte-Carlo)
  - many random effects per individual => large integration dimension:

    Monte-Carlo to be preferred
- To eliminate the hidden process we can perform forward-backward (when taking the expectation in EM), or simply forward (when integrating in likelihood approximation).

# Perspectives (of my PhD thesis)

- oconsider HSMMs (with a general model)
- implement some available methods (Monte-Carlo, quadrature, variationnal EM, Newton-Raphson, etc.)
- compare estimation methods

- [1] Haji-Maghsoudi et al. "Generalized linear mixed hidden semi-Markov models in longitudinal set-tings: A Bayesian approach". In: (2021).
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- [6] Maruotti. "Mixed Hidden Markov Models for Longitudinal Data : An Overview". In: (2011).
- [7] Michelot. "hmmTMB: Hidden Markov models with flexible covariate effects in". In: (2023).