

# Multiple Trajectory Analysis in Finite Mixture Modeling

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joint work with

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ASMDA 2021

June 2, 2021

# Outline

## 1 Finite Mixture Models

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# General description of Nagin's model

We have a collection of individual trajectories.

We try to divide the population into a number of homogenous sub-populations and to estimate, at the same time, a typical trajectory for each sub-population.

Hence, this model can be interpreted as functional fuzzy cluster analysis.

Finite mixture model (Daniel S. Nagin (Carnegie Mellon University))

- mixture : population composed of a mixture of unobserved groups
- finite : sums across a finite number of groups



# The Likelihood Function (1)

Consider a population of size  $N$  and a variable of interest  $Y$ .

Let  $Y_i = y_{i1}, y_{i2}, \dots, y_{iT}$  be  $T$  measures of the variable, taken at times  $t_1, \dots, t_T$  for subject number  $i$ .  $A_i = \{t_1, \dots, t_T\}$

$\pi_k$  : probability of a given subject to belong to group number  $k$

$\Rightarrow \pi_k$  is the size of group  $k$ .

$$\Rightarrow P(Y_i) = \sum_{k=1}^K \pi_k P^k(Y_i), \quad (1)$$

where  $P^k(Y_i)$  is probability of  $Y_i$  if subject  $i$  belongs to group  $k$ .

## The Likelihood Function (2)

Aim of the analysis: Find  $K$  groups of trajectories of a given kind, for instance polynomials of degree 4,  $P(t) = \beta_0 + \beta_1 t + \beta_2 t^2 + \beta_3 t^3 + \beta_4 t^4$ .

Statistical Model:

$$y_{it} = \beta_0^k + \beta_1^k t + \beta_2^k t^2 + \beta_3^k t^3 + \beta_4^k t^4 + \varepsilon_{it}^k, \quad (2)$$

where  $\varepsilon_{it}^k \sim \mathcal{N}(0, \sigma_k)$ ,  $\sigma_k$  being the standard deviation, constant inside group  $k$ .

We try to estimate a set of parameters  $\Omega = \{\beta_0^k, \beta_1^k, \beta_2^k, \beta_3^k, \beta_4^k, \pi_k, \sigma_k\}$  which allow to maximize the probability of the measured data.

# Possible data distributions

- count data  $\Rightarrow$  Poisson distribution
- binary data  $\Rightarrow$  Binary logit distribution
- censored data  $\Rightarrow$  Censored normal distribution

## Predictors of trajectory group membership

$x$  : vector of variables potentially associated with group membership (measured before  $t_1$ ).

Multinomial logit model:

$$\pi_k(x_i) = \frac{e^{x_i\theta_k}}{\sum_{k=1}^K e^{x_i\theta_k}}, \quad (3)$$

where  $\theta_k$  denotes the effect of  $x_i$  on the probability of group membership for group  $k$ .

$$L = \prod_{i=1}^N \sum_{k=1}^K \frac{e^{x_i\theta_k}}{\sum_{k=1}^K e^{x_i\theta_k}} \prod_{t=1}^T p^k(y_{it}), \quad (4)$$

where  $p^k(\cdot)$  denotes the distribution of  $y_{it}$  conditional on membership in group  $k$ .

## Adding covariates to the trajectories

Let  $W$  be a vector of covariates potentially influencing  $Y$ .

The likelihood then becomes

$$L = \prod_{i=1}^N \sum_{k=1}^K \frac{e^{x_i \theta_k}}{\sum_{k=1}^K e^{x_i \theta_k}} \prod_{t=1}^T p^k(y_{it} | A_i, W_i, \Theta_k).$$

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# Basic Idea

We conjointly analysis the trajectories of  $J$  variables  $Y^1, \dots, Y^J$ .

# The constrained model

We suppose the existence of  $K$  unique groups representing the combined development of  $Y^j$ ,  $1 \leq j \leq J$ .

The conditional independence of the time measurements for the outcomes for a given group is implies that

$$P(Y_i^1, \dots, Y_i^J | A_i, W_i) = \sum_{k=1}^K \pi_k \prod_{j=1}^J \prod_{t=1}^T p^k(y_{it}^j | A_i, W_i, \Theta_k^j).$$



## The unconstrained model

We suppose the trajectories for a variable  $Y^l$  can be linked to trajectories for all other variables  $Y^j, j \neq l$ . Then,

$$P(Y_i^1, \dots, Y_i^J | A_i, W_i) = \sum_{(k_1, \dots, k_J) \in K_1 \times \dots \times K_J} \pi_{k_J | k_1 \dots k_{J-1}} \times \dots \times \pi_{k_2 | k_1} \times \pi_{k_1} \\ \prod_{j=1}^J \prod_{t=1}^T p^{k_j}(y_{it}^j | A_i, W_i, \Theta_k^j),$$

where  $\pi_{k_j | k_1 \dots k_{j-1}}$  is the probability of belonging to group  $j$  conditional on the membership to groups 1 to  $j - 1$ .

# Membership Probability

$$\pi_{k_1} = \frac{e^{\theta_{k_1} x_i}}{\sum_{k_1=1}^{K_1} e^{\theta_{k_1} x_i}}, \quad \pi_{k_2|k_1} = \frac{e^{\theta_{k_2}^{k_1} w_i^{k_2}}}{\sum_{k_2=1}^{K_2} e^{\theta_{k_2}^{k_1} w_i^{k_2}}}, \quad \dots,$$
$$\pi_{k_J|k_1 \dots k_{J-1}} = \frac{e^{\theta_{k_J}^{k_1 \dots k_{J-1}} w_i^{k_J}}}{\sum_{k_J=1}^{K_J} e^{\theta_{k_J}^{k_1 \dots k_{J-1}} w_i^{k_J}}}.$$

One drawback of this method is the great expansion of the number of parameters and the fact that the parameters are hardly interpretable.

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## Group Membership Vector

Denote by  $Z_i = (Z_{i1}, \dots, Z_{iJ})$  the vector containing the group membership of individual  $i$  for the variables  $Y^1, \dots, Y^J$ .  $Z_i \in \llbracket 1; K_1 \rrbracket \times \dots \times \llbracket 1; K_J \rrbracket$ .

Then,

$$P\left(Z_{ij} = k \mid z_{ih} \text{ for } h \neq j, X_i^j\right) = \frac{e^{B_{ij,k}}}{\sum_{h=1}^{K_j} e^{B_{ij,h}}},$$

where  $B_{ij,k} = \alpha_{j,k} + \beta_{j,k} X_i^j + \sum_{h \neq j} \psi_{jh,kz_{ih}}$ .

- $\alpha_{j,k}$  is a choice specific intercept ;
- $\beta_{j,k}$  is a vector corresponding to the covariate  $X_i^j$  ;
- $z_{ih}$  the group membership of the individual  $i$  for  $Y^h$  ;
- $\psi_{jh,kl}$  is an association parameter between belonging to group  $k$  for  $Y^j$  and belonging to the group  $l$  for  $Y^h$ .

## Number of parameters

The Hammersley-Clifford Theorem allows to write the conditional probabilities as

$$P\left(Z_{ij} = k \mid z_{ih} \text{ for } h \neq j, X_i^j\right) = \frac{e^{B_{ij,k}}}{\sum_{h=1}^{K_j} e^{B_{ij,h}}}$$

where  $B_{ij,k} = \alpha_{j,k} + \beta_{j,k} X_i^j + \sum_{h < j} \psi_{hj, z_{ih} k} + \sum_{h > j} \psi_{jh, k z_{ih}}$ .

### Proposition

The numbers of parameters is

$$\sum_{j=1}^J (K_j - 1) \times (\text{ncol}(X_i^j) + 1) + \sum_{1 \leq j \neq j' \leq J} (K_j - 1)(K_{j'} - 1).$$

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# Setup

We simulate trajectories for 200 individuals and 3 variables.

- $Y^1$  (normal distribution) :  $\beta_{1,1} = (3.53, -2.25, 0.47)$ ,  
 $\beta_{1,2} = (-1.62, 3.9, -0.65)$ ,  $\beta_{1,3} = (0.263, 0.036, 0.01)$ ,  
 $\sigma_{1,1} = \sigma_{1,2} = \sigma_{1,3} = 1$  ;
- $Y^2$  (ZIP distribution) :  $\beta_{2,1} = (1.2, 2.3, -1.2, 0.5, -0.1)$ ,  $\beta_{2,2} = (2)$ ,  
 $\beta_{2,3} = (-7.5, 0, 2.2, -.4)$ ,  $\nu_1 = (-2, 1)$ ,  $\nu_2 = (-1, 0.1)$ ,  $\nu_3 = (0, -1)$ ;
- $Y^3$  (logit distribution) :  $\beta_{3,1} = (6.32, -5.8, 1)$ ,  $\beta_{3,2} = (-6.69, 1.92)$ .

Furthermore, we choose all  $\theta_{j,k} = 0$  and  $\psi = (-3, 3, 4, 0, -2, 5, 1, 0)$ . We launch trajER for each variable separately and we use the results as initial values for the multi-trajectory model.

# Results

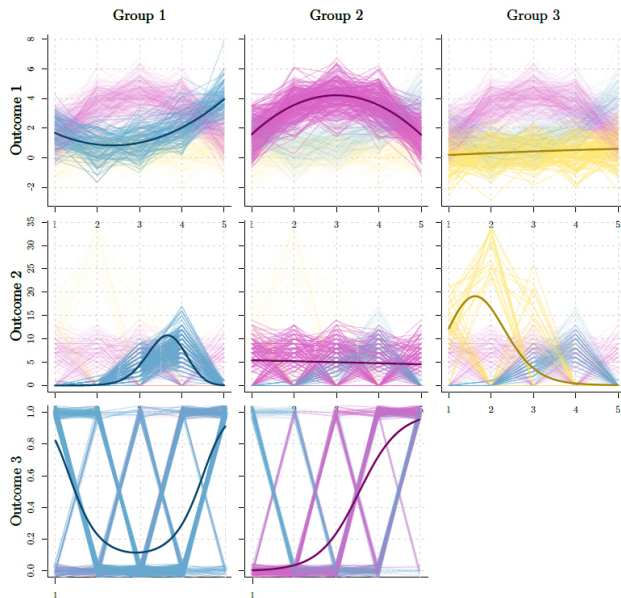
	Variable 1				Variable 2		
	Th.	EM	L		Th.	EM	L
$\beta_{11}$	3.53	3.37162	3.37154	$\beta_{11}$	1.2	-3.92980	-3.92950
$\beta_{12}$	-2.25	-2.13530	-2.13523	$\beta_{12}$	2.3	-4.11672	-4.11653
$\beta_{13}$	0.47	0.45090	0.45089	$\beta_{13}$	-1.2	3.88076	3.88051
$\beta_{21}$	-1.620	-1.71513	-1.71513	$\beta_{14}$	0.5	-0.68312	-0.68305
$\beta_{22}$	3.900	3.96422	3.96422	$\beta_{15}$	-0.1	0.01616	0.01615
$\beta_{23}$	-0.650	-0.66183	-0.66183	$\beta_{21}$	2	2.01483	2.01483
$\beta_{31}$	0.263	0.04619	0.04624	$\beta_{31}$	-7.5	-0.39232	-0.39204
$\beta_{32}$	0.036	0.15730	0.15725	$\beta_{32}$	0	4.55945	4.55895
$\beta_{33}$	0.010	-0.00882	-0.00881	$\beta_{33}$	2.2	-1.69650	-1.69623
$\sigma$	1	2.69943	2.69943	$\beta_{34}$	-0.4	0.17702	0.17698
$\theta_1$	0	0.00000	0.00000	$\nu_{11}$	-2	-0.98558	-0.98296
$\theta_2$	0	2.00645	2.00672	$\nu_{12}$	1	-0.7915	-0.79232
$\theta_3$	0	-5.40659	-5.43048	$\nu_{21}$	-1	-1.08749	-1.08734
				$\nu_{22}$	0.1	0.13039	0.13035
				$\nu_{31}$	0	-3.38530	-3.38515
				$\nu_{32}$	-1	1.53658	1.53652
				$\theta_1$	0	0.00000	0.00000
				$\theta_2$	0	-0.07507	-0.07461
				$\theta_3$	0	0.14593	0.14628

	Variable 3		
	Th.	EM	L
$\beta_{11}$	6.32	6.28035	6.28024
$\beta_{12}$	-5.8	-5.73551	-5.73545
$\beta_{13}$	1	0.98963	0.98962
$\beta_{21}$	-6.69	-7.46613	-7.46609
$\beta_{22}$	1.92	2.09930	2.09930
$\theta_1$	0	0.00000	0.00000
$\theta_2$	0	-2.09538	-2.09295

Parameters	$\psi_{12,22}$	$\psi_{12,23}$	$\psi_{12,32}$	$\psi_{12,33}$	$\psi_{13,22}$	$\psi_{13,32}$	$\psi_{23,22}$	$\psi_{23,32}$
Theoretical	-3	3	4	0	-2	5	1	0
EM	-5.47292	4.33422	-4.57086	-4.46658	-2.12297	3.23218	1.18008	-7.96007
Likelihood	-5.46968	4.35722	-4.57081	-3.3298	-2.12013	3.23351	1.17703	-10.00915



# Results



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# Montreal Longintudinal Study

Example from D. Nagin. Compares the link between hyperactivity and opposition score. The hyperactivity is measured on a scale between 0 and 4 and the opposition behavior on a scale between 0 and 10.

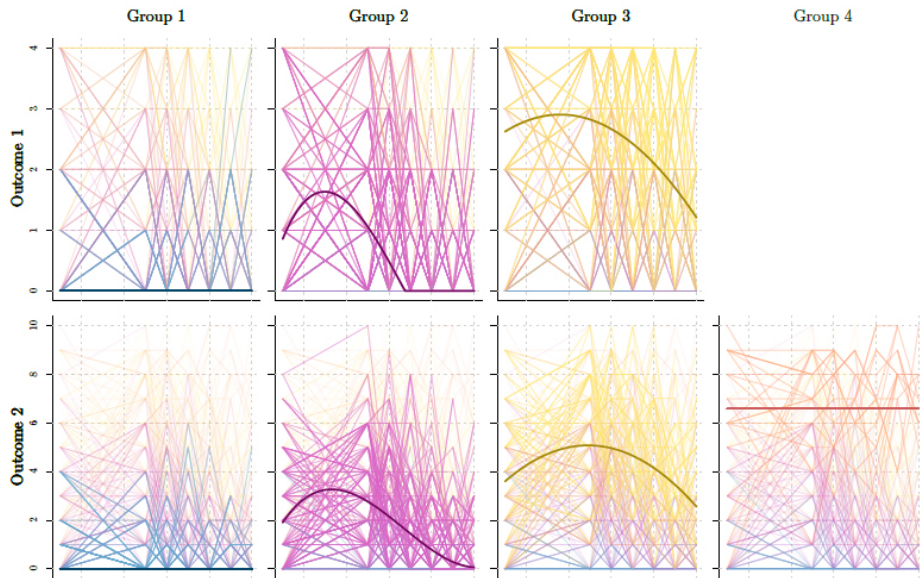
# Results

	Variable 1			Variable 2	
	TrajeR	traj (SAS)		TrajeR	traj (SAS)
$\beta_{11}$	-2.55343	-2.55348	$\beta_{11}$	-1.67252	-1.67258
$\beta_{21}$	0.48071	0.48074	$\beta_{12}$	-1.48300	-1.48308
$\beta_{22}$	-6.24514	-6.24425	$\beta_{21}$	2.15443	2.15440
$\beta_{23}$	-3.53665	-3.53676	$\beta_{22}$	-6.79570	-6.79186
$\beta_{24}$	14.90876	14.90347	$\beta_{23}$	-4.29020	-4.29356
$\beta_{31}$	2.66416	2.66411	$\beta_{24}$	20.58775	20.56512
$\beta_{32}$	-1.98842	-1.98840	$\beta_{31}$	4.96622	4.96615
$\beta_{33}$	-4.14192	-4.14164	$\beta_{32}$	-2.12531	-2.12503
$\sigma$	2.31949	2.3195	$\beta_{33}$	-9.72094	-9.71914
			$\beta_{41}$	6.59242	6.59246
			$\sigma$	2.54359	2.5436

With `trajeR` we find the following 6 linking parameters.

Parameters	$\psi_{12,22}$	$\psi_{12,23}$	$\psi_{12,24}$	$\psi_{12,32}$	$\psi_{12,33}$	$\psi_{12,34}$
Theoretical	19.97949	10.51569	8.94481	28.44746	31.69029	40.0845

# Results



# Bibliography

- Nagin, D.S. 2005: *Group-based Modeling of Development*. Cambridge, MA.: Harvard University Press.
- Schiltz, J. 2015: A generalization of Nagin's finite mixture model. In: Dependent data in social sciences research: Forms, issues, and methods of analysis' Mark Stemmler, Alexander von Eye & Wolfgang Wiedermann (Eds.). Springer 2015.
- Nagin, D.S., Jones, B.L., Lima Passos, V. & Tremblay, R.E. 2018: Group-based multi-trajectory modeling. *Statistical Methods in Medical Research*, 27-7.
- Noel, C & Schiltz, J. 2021: TrajeR - an R package for finite mixture models.
- Noel, C & Schiltz, J. 2021: A new algorithm for group-based multi-trajectory modeling.