Drifting semi-Markov models: Estimation and Simulation through the dsmmR package

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Plan

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Definition (linear drifting Markov chain of order 1 and of length $n$)

A sequence $X_0, X_1, \ldots, X_n$ with state space $E = \{1, 2, \ldots, s\}$ is called a **linear drifting Markov chain (of order 1)** of length $n$ between the Markov transition matrices $\Pi_0$ and $\Pi_1$, if the distribution of $X_t$, $t = 1, \ldots, n$, is defined by

$$
P(X_t = v \mid X_{t-1} = u) = \Pi_{\frac{t}{n}}(u, v), \ u, v \in E,
$$

where $\Pi_{\frac{t}{n}}(u, v) = \left(1 - \frac{t}{n}\right) \Pi_0(u, v) + \frac{t}{n} \Pi_1(u, v), \ u, v \in E$.

Estimation method: Least squares estimators. We minimize

$$
\sum_{t=1}^{n} \sum_{u \in E} \sum_{v \in E} 1 \{X_{t-1} = u\} \left(\Pi_{\frac{t}{n}}(u, v) - 1 \{X_t = v\}\right)^2.
$$
Polynomial drifting Markov model

Definition (polynomial drifting Markov chain of order $k$ and of length $n$)

A sequence $X_0, X_1, \ldots, X_n$ with state space $E = \{1, 2, \ldots, s\}$ is said to be a polynomial drifting Markov chain of order $k$ and of length $n$ if the distribution of $X_t$, $t = 1, \ldots, n$, is defined for $u_1, \ldots, u_k, v \in E$ by

$$
P(X_t = v \mid X_{t-1} = u_k, X_{t-2} = u_{k-1}, \ldots) = \Pi_{\frac{t}{n}}(u_1, \ldots, u_k, v)
$$

where

$$
\Pi_{\frac{t}{n}}(u_1, \ldots, u_k, v) = \sum_{i=0}^d A_i(t) \prod_{\frac{i}{d}}(u_1, \ldots, u_k, v)
$$

with $A_i$ polynomials of degree $d$ such as, for any $i, j \in \{0, 1, \ldots, d\}$,

$$
A_i \left(\frac{n_j}{d}\right) = 1_{\{i=j\}}.
$$

Note: for $t = ni/d$, we have $\Pi_{\frac{t}{n}} = \Pi_{\frac{i}{d}}$.

Remark ($A_i$ are Lagrange polynomials: chosen to have stochastic $\Pi_{\frac{t}{n}}$)

Indeed

$$
\sum_{v \in E} \Pi_{\frac{t}{n}}(u_1, \ldots, u_k, v) = \sum_{i=0}^d A_i(t) = A(t) \text{ where } A \text{ is a polynomial of degree } d \text{ equal to one in } (d + 1) \text{ points; then } A \text{ is a constant polynomial equal to one.}$$
Proposition

Let \( 1_u := 1\{X_{t-k} \ldots X_{t-1} = u_1 \ldots u_k\} \) and \( 1_{uv} := 1\{X_{t-k} \ldots X_{t-1} = u_1 \ldots u_k, X_t = v\} \). For \((X_0, X_1, \ldots, X_n)\) a sample path of a polynomial drifting Markov chain of order \( k \) and degree \( d \), for any states \( u_1, \ldots, u_k, v \in E \), the estimators of \( \Pi_{id}(u_1, \ldots u_k, v) \) are given by solving the following linear system

\[
\begin{pmatrix}
\sum_{t=k}^{n} 1_u A_0(t) A_0(t) & \cdots & \sum_{t=k}^{n} 1_u A_0(t) A_d(t) \\
\vdots & \ddots & \vdots \\
\sum_{t=k}^{n} 1_u A_d(t) A_0(t) & \cdots & \sum_{t=k}^{n} 1_u A_d(t) A_d(t)
\end{pmatrix}
\begin{pmatrix}
\Pi_0; n \\
\vdots \\
\Pi_1; n \\
\vdots \\
\Pi_d; n
\end{pmatrix}
= \begin{pmatrix}
\sum_{t=k}^{n} A_0(t) 1_{uv} \\
\vdots \\
\sum_{t=k}^{n} A_d(t) 1_{uv}
\end{pmatrix}.
\]
Fréquences / Lois stationnaires (degré 1) sur *Chlamydia trachomatis*

![Graphs showing distributions of various characters](image-url)
Fréquences / Lois stationnaires (degré 2)
Fréquences / Lois stationnaires (degré 3)
Fréquences / Lois stationnaires (degré 4)
Fréquences / Lois stationnaires (degré 5)

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Fréquences / Lois stationnaires (degré 8)
Software, R Package, Web Interface and Applications


1. Thanks to FEDER DAISI
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Different chains

- $Z = (Z_k)_{k \in \mathbb{N}}$, chain with state space $E = \{1, 2, \ldots, s\}$
- $S = (S_n)_{n \in \mathbb{N}}$, jump times
- $J = (J_n)_{n \in \mathbb{N}}$, visited states
- $X = (X_n)_{n \in \mathbb{N}}$, sojourn times of $Z$
the initial distribution $\alpha(i) := \mathbb{P}(J_0 = i)$

the homogeneous SM kernel $\mathbf{q} = (q(i, j; k))_{i, j \in E, k \in \mathbb{N}}$

$$q(i, j; k) := \begin{cases} \mathbb{P}(J_{n+1} = j, X_{n+1} = k | J_n = i), & k \in \mathbb{N}^* \\ 0, & k = 0 \end{cases}$$

the conditional sojourn time distributions $\mathbf{f} = (f(i, j; k))_{i, j \in E, k \in \mathbb{N}}$

$$f(i, j; k) := \mathbb{P}(X_{n+1} = k | J_n = i, J_{n+1} = j), \quad f(i, j; 0) := 0$$

the transition matrix of the MC $(J_n)_{n \in \mathbb{N}}, \quad \mathbf{p} = (p(i, j))_{i, j \in E}$

$$p(i, j) := \mathbb{P}(J_{n+1} = j | J_n = i), \quad p(i, i) := 0$$

Note that $q(i, j; k) = p(i, j) f(i, j; k)$


2. Thanks to RIN Asterics and FEDER DAISI
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Definition (linear drifting semi-Markov chain of length $n$ – Model 1)

A sequence $Z_0, Z_1, \ldots, Z_{N(n)}$ with state space $E = \{1, 2, \ldots, s\}$ is called a linear drifting Markov chain of length $n$ of Model 1 between the semi-Markov kernels $q_0$ and $q_1$, if for $t = 0, \ldots, n$, we have

$$
\mathbb{P}(J_{t+1} = v, S_{t+1} - S_t = \ell | J_t = u) = q_{\frac{t}{n}}(u, v, \ell),
$$

where $q_{\frac{t}{n}}(u, v, \ell) = \left(1 - \frac{t}{n}\right)q_0(u, v, \ell) + \frac{t}{n}q_1(u, v, \ell)$, $u, v \in E, \ell \in \mathbb{N}$. 

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Definition (linear drifting semi-Markov chain of length $n$ – Model 2)

A sequence $Z_0, Z_1, \ldots, Z_{N(n)}$ with state space $E = \{1, 2, \ldots, s\}$ is called a linear drifting Markov chain of length $n$ of Model 2 between the semi-Markov kernels $q_0$ and $q_1$, if for $t = 0, \ldots, n$, we have

$$P(J_{t+1} = v, S_{t+1} - S_t = \ell | J_t = u) = q_{\frac{t}{n}}(u, v, \ell),$$

where

$$q_{\frac{t}{n}}(u, v; \ell) = \left(1 - \frac{t}{n}\right)f(u, v; \ell)p_0(u, v) + \frac{t}{n}f(u, v; \ell)p_1(u, v),$$

with $p_0$ and $p_1$ Markov kernels, $f(u, v; \ell)$ the conditional distribution of the sojourn in state $u$ before jumping to $v$ equal to $\ell$. 
Definition (linear drifting semi-Markov chain of length $n$ – Model 3)

A sequence $Z_0, Z_1, \ldots, Z_{N(n)}$ with state space $E = \{1, 2, \ldots, s\}$ is called a linear drifting Markov chain of length $n$ of Model 3 between the semi-Markov kernels $q_0$ and $q_1$, if for $t = 0, \ldots, n$, we have

$$
\mathbb{P}(J_{t+1} = v, S_{t+1} - S_t = \ell | J_t = u) = q_{\frac{t}{n}}(u, v, \ell), \text{ where}
$$

$$
q_{\frac{t}{n}}(u, v; \ell) = \left(1 - \frac{t}{n}\right) f_0(u, v, \ell)p(u, v) + \frac{t}{n} f_1(u, v, \ell)p(u, v),
$$

with $p$ a Markov kernel, $f_0(u, v; \ell)$ and $f_1(u, v; \ell)$ conditional distributions of the sojourn in state $u$ before jumping to $v$ equal to $\ell$. 

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Drifting semi-Markov models: dsmmR package

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Polynomial DSMM

Model 1: \textbf{\textit{p and f are drifting}}. The DSM kernel is given by:

\[
q_{\frac{1}{n}}^{(1)} = \sum_{i=0}^{d} A_i(t)q_{\frac{1}{d}}^{(1)}(u,v,l) = \sum_{i=0}^{d} A_i(t)p_{\frac{i}{d}}(u,v)f_{\frac{i}{d}}(u,v,l)
\]

Model 2: \textbf{\textit{Only p is drifting}} (\(f\) is not drifting). The DSM kernel is given by:

\[
q_{\frac{2}{n}}^{(2)}(u,v,l) = \sum_{i=0}^{d} A_i(t)q_{\frac{2}{d}}^{(2)}(u,v,l) = \sum_{i=0}^{d} A_i(t)p_{\frac{i}{d}}(u,v)f(u,v,l)
\]

Model 3: \textbf{\textit{Only f is drifting}} (\(p\) is not drifting). The DSM kernel is given by:

\[
q_{\frac{3}{d}}^{(3)}(u,v,l) = \sum_{i=0}^{d} A_i(t)q_{\frac{3}{d}}^{(3)}(u,v,l) = \sum_{i=0}^{d} A_i(t)p(u,v)f_{\frac{i}{d}}(u,v,l)
\]
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Non-parametric Estimation for model 1

Model 1

We can estimate the DSM kernel by Least Square Estimation (LSE),

$$\hat{q}_{i}^{(1)}(u, v, l) = \sum_{i=0}^{d} A_i(t) \hat{q}_{i}^{(1)}(u, v, l)$$

∀u, v ∈ E, l ∈ {1, ..., k_{max}}, where k_{max} is the maximum realized sojourn time in the sequence, we obtain the SM kernels $\hat{q}_{i}^{(1)}(u, v, l), i = 0, ..., d$.

Estimators of $\hat{p}_{i}(u, v)$ and $\hat{f}_{i}^{d}(u, v, l)$ are obtained as in SMM:

$$\hat{p}_{i}^{d}(u, v) = \sum_{l=1}^{k_{max}} \hat{q}_{i}^{d}(u, v, l),$$

$$\hat{f}_{i}^{d}(u, v, l) = \frac{\hat{q}_{i}^{d}(u, v, l)}{\sum_{l=1}^{k_{max}} \hat{q}_{i}^{d}(u, v, l)} = \frac{\hat{q}_{i}^{d}(u, v, l)}{\hat{p}_{i}^{d}(u, v)}.$$
Non-parametric Estimation for model 1

Model 1: we solve $MJ = P$ to obtain $\hat{q}^{(1)}_{id}(u, v, l)$

$$M = \begin{pmatrix}
\sum_{t=1}^{n} 1_{u(t)}A_0(t)A_0(t) & \cdots & \sum_{t=1}^{n} 1_{u(t)}A_0(t)A_d(t) \\
\vdots & \ddots & \vdots \\
\sum_{t=1}^{n} 1_{u(t)}A_d(t)A_0(t) & \cdots & \sum_{t=1}^{n} 1_{u(t)}A_d(t)A_d(t)
\end{pmatrix}$$

$$J = \begin{pmatrix}
\hat{q}^{(1)}_{0}(u, v, l) \\
\vdots \\
\hat{q}^{(1)}_{i}(u, v, l) \\
\hat{q}^{(1)}_{1}(u, v, l)
\end{pmatrix}$$

and

$$P = \begin{pmatrix}
\sum_{t=1}^{n} 1_{uvl}(t)A_0(t) \\
\vdots \\
\sum_{t=1}^{n} 1_{uvl}(t)A_i(t) \\
\sum_{t=1}^{n} 1_{uvl}(t)A_1(t)
\end{pmatrix}$$

Where $1_{u(t)} = 1\{J_{t-1}=u\}(t)$, and $1_{uvl}(t) = 1\{J_t=v, J_{t-1}=u, X_t=l\}(t)$. 
Non-parametric Estimation for model 2

Model 2

\[
\hat{p}_{id}(u, v) = \sum_{l=1}^{k_{\text{max}}} \hat{q}_{id}^{(1)}(u, v, l) \quad \text{(as in Model 1)}
\]

\[
\hat{f}(u, v, l) = \frac{\sum_{i=0}^{d} \hat{q}_{id}^{(1)}(u, v, l)}{\sum_{i=0}^{d} \sum_{l=1}^{k_{\text{max}}} \hat{q}_{id}^{(1)}(u, v, l)}, \quad \text{with} \quad \sum_{l=1}^{k_{\text{max}}} \hat{f}(u, v, l) = 1
\]

This leads to the estimated SM kernel for Model 2 \(\hat{q}_{id}^{(2)}(u, v, l)\) being described through model 1:

\[
\hat{q}_{id}^{(2)}(u, v, l) = \frac{\left(\sum_{i=1}^{k_{\text{max}}} \hat{q}_{id}^{(1)}(u, v, l)\right) \left(\sum_{i=0}^{d} \hat{q}_{id}^{(1)}(u, v, l)\right)}{\sum_{i=0}^{d} \sum_{l=1}^{k_{\text{max}}} \hat{q}_{id}^{(1)}(u, v, l)}
\]
Non-parametric Estimation for model 3

Model 3

\[
\hat{p}(u, v) = \frac{\sum_{i=0}^{d} \sum_{l=1}^{k_{max}} \hat{q}^{(1)}_{i d}(u, v, l)}{d + 1}, \quad \text{with} \quad \sum_{v \in E} \hat{p}(u, v) = 1
\]

\[
\hat{f}^{(1)}_{i d}(u, v, l) = \frac{\hat{q}^{(1)}_{i d}(u, v, l)}{\sum_{l=1}^{k_{max}} \hat{q}^{(1)}_{i d}(u, v, l)} \quad \text{(as in model 1)}.
\]

This leads to the estimated SM kernel for \textbf{Model 3} \( \hat{q}^{(3)}_{i d}(u, v, l) \) being described through model 1:

\[
\hat{q}^{(3)}_{i d}(u, v, l) = \frac{\hat{q}^{(1)}_{i d}(u, v, l) \sum_{i=0}^{d} \sum_{l=1}^{k_{max}} \hat{q}^{(1)}_{i d}(u, v, l)}{(d + 1) \sum_{l=1}^{k_{max}} \hat{q}^{(1)}_{i d}(u, v, l)}
\]
In conclusion:

Model 1

\[
\hat{q}_{t/n}^{(1)}(u, v, l) = \sum_{i=0}^{d} A_i \hat{q}_{d}^{(1)}(u, v, l)
\]

Model 2

\[
\hat{q}_{t/n}^{(2)}(u, v, l) = \sum_{i=0}^{d} A_i(t) \left( \frac{\sum_{l=1}^{k_{max}} \hat{q}_{d}^{(1)}(u, v, l)}{\sum_{i=0}^{d} \sum_{l=1}^{k_{max}} \hat{q}_{d}^{(1)}(u, v, l)} \right) \left( \sum_{i=0}^{d} \hat{q}_{d}^{(1)}(u, v, l) \right) \]

Model 3

\[
\hat{q}_{t/n}^{(3)}(u, v, l) = \sum_{i=0}^{d} A_i(t) \left( \hat{q}_{d}^{(1)}(u, v, l) \sum_{i=0}^{d} \sum_{l=1}^{k_{max}} \hat{q}_{d}^{(1)}(u, v, l) \right) \left( (d + 1) \sum_{l=1}^{k_{max}} \hat{q}_{d}^{(1)}(u, v, l) \right)
\]
Estimators of parameters for the discrete distribution of sojourn time

We note \( \hat{m}_1 = \sum_{x=1}^{k_{max}} x \hat{f}(x) \) and \( \hat{m}_2 = \sum_{x=1}^{k_{max}} x^2 \hat{f}(x) - \hat{m}_1^2 \).

- **Geometric** \((p)\) : \( f(x) = p(1 - p)^{x-1}, x = 1, \ldots, k_{max} \). Then \( \hat{p} = 1/\hat{m}_1 \).

- **Poisson** \((\lambda)\) : \( f(x) = \frac{\lambda^{x-1} \exp(-\lambda)}{(x-1)!}, x = 1, \ldots, k_{max} \). Then \( \hat{\lambda} = \hat{m}_1 \).

- **Negative Binomial** \((\alpha, p)\) : \( f(x) = \frac{\Gamma(x+\alpha-1)}{\Gamma(\alpha)(x-1)!} p^\alpha (1 - p)^{x-1}, x = 1, \ldots, k_{max} \). Therefore:

  \[
  \hat{p} = \frac{\hat{m}_1}{\hat{m}_2}, \quad \hat{\alpha} = \hat{m}_1 \frac{\hat{p}}{1-\hat{p}} = \frac{\hat{m}_1^2}{\hat{m}_2 - \hat{m}_1}
  \]

- **Discrete Weibull** \((q, \beta)\) : \( f(x) = q^{(x-1)\beta} - q^{x\beta}, x = 1, \ldots, k_{max} \). Therefore:

  \[
  \hat{q} = 1 - \hat{f}(1), \quad \hat{\beta} = \frac{\sum_{i=2}^{k_{max}} \log_i (\log_q (\sum_{j=1}^{i} \hat{f}(j)))}{k_{max} - 1}
  \]
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It constitutes of the main functions:

1. `fit_dsmm()`:
   Fit a DSMM on a given sequence. Parametric or non-parametric estimation is possible (Model 1, 2 or 3).

2. `parametric_dsmm()` & `nonparametric_dsmm()`:
   Define a parametric or non-parametric DSMM (Model 1, 2 or 3).

3. `simulate.dsmm()`:
   Generate a sequence of states with a maximum number of simulations equal to \( n + 1 \) (model size).

4. `get_kernel()`:
   Compute the DSM kernel \( q_{\frac{t}{n}} \).
$d + 1$ Sojourn Time Distributions: $f_0$, $f_{\frac{1}{2}}$ and $f_1$

<table>
<thead>
<tr>
<th>$f_0(u,v,l = 1)$</th>
<th>$f_{\frac{1}{2}}(u,v,l = 1)$</th>
<th>$f_1(u,v,l = 1)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$=$</td>
<td>$=$</td>
<td>$=$</td>
</tr>
<tr>
<td>$\begin{pmatrix} 0 &amp; 0.2 &amp; 0.7 \ 0.3 &amp; 0 &amp; 0.4 \ 0.2 &amp; 0.8 &amp; 0 \end{pmatrix}$</td>
<td>$\begin{pmatrix} 0 &amp; 0.3333333 &amp; 0.4 \ 0.3 &amp; 0 &amp; 0.4 \ 0.2 &amp; 0.1 &amp; 0 \end{pmatrix}$</td>
<td>$\begin{pmatrix} 0 &amp; 0.3 &amp; 0.3 \ 0.3 &amp; 0 &amp; 0.5 \ 0.05 &amp; 0.1 &amp; 0 \end{pmatrix}$</td>
</tr>
<tr>
<td>$f_0(u,v,l = 2)$</td>
<td>$f_{\frac{1}{2}}(u,v,l = 2)$</td>
<td>$f_1(u,v,l = 2)$</td>
</tr>
<tr>
<td>$=$</td>
<td>$=$</td>
<td>$=$</td>
</tr>
<tr>
<td>$\begin{pmatrix} 0 &amp; 0.3 &amp; 0.2 \ 0.2 &amp; 0 &amp; 0.5 \ 0.1 &amp; 0.15 &amp; 0 \end{pmatrix}$</td>
<td>$\begin{pmatrix} 0 &amp; 0.3333333 &amp; 0.4 \ 0.4 &amp; 0 &amp; 0.2 \ 0.3 &amp; 0.4 &amp; 0 \end{pmatrix}$</td>
<td>$\begin{pmatrix} 0 &amp; 0.2 &amp; 0.6 \ 0.3 &amp; 0 &amp; 0.35 \ 0.9 &amp; 0.2 &amp; 0 \end{pmatrix}$</td>
</tr>
<tr>
<td>$f_0(u,v,l = 3)$</td>
<td>$f_{\frac{1}{2}}(u,v,l = 3)$</td>
<td>$f_1(u,v,l = 3)$</td>
</tr>
<tr>
<td>$=$</td>
<td>$=$</td>
<td>$=$</td>
</tr>
<tr>
<td>$\begin{pmatrix} 0 &amp; 0.5 &amp; 0.1 \ 0.5 &amp; 0 &amp; 0.1 \ 0.7 &amp; 0.05 &amp; 0 \end{pmatrix}$</td>
<td>$\begin{pmatrix} 0 &amp; 0.3333333 &amp; 0.2 \ 0.3 &amp; 0 &amp; 0.4 \ 0.5 &amp; 0.5 &amp; 0 \end{pmatrix}$</td>
<td>$\begin{pmatrix} 0 &amp; 0.5 &amp; 0.1 \ 0.4 &amp; 0 &amp; 0.15 \ 0.05 &amp; 0.7 &amp; 0 \end{pmatrix}$</td>
</tr>
</tbody>
</table>
$d + 1$ Transition Matrices - $p_0, p_{\frac{1}{2}}$ and $p_1$ and metric

\[
\begin{bmatrix}
p_0(u, v) = \\
(0 & 0.1 & 0.9) \\
(0.5 & 0 & 0.5) \\
(0.3 & 0.7 & 0) \\
\end{bmatrix}
\begin{bmatrix}
p_{\frac{1}{2}}(u, v) = \\
(0 & 0.6 & 0.4) \\
(0.7 & 0 & 0.3) \\
(0.6 & 0.4 & 0) \\
\end{bmatrix}
\begin{bmatrix}
p_1(u, v) = \\
(0 & 0.2 & 0.8) \\
(0.6 & 0 & 0.4) \\
(0.7 & 0.3 & 0) \\
\end{bmatrix}
\]

We are going to use the following metric, defining the distance between the $d + 1$ theoretical kernels $q^{(M)}_i$ with the estimated ones $\hat{q}^{(M)}_i$, for all 3 models $M = 1, 2, 3$:

\[
d\left(q^{(M)}_i, \hat{q}^{(M)}_i\right) = \sum_{u,v,l} \left(q^{(M)}_i - \hat{q}^{(M)}_i\right)^2,
\]

where $u, v \in E, l \in \{1, \ldots, k_{max}\}$.
SM Kernels differences for Model 1

- $J_0$
- $J_{1/2}$
- $J_1$
SM Kernels differences for Model 2

![Graph showing differences for Model 2 with lines for J_0, J_1/2, and J_1.]

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Concluding remarks

Conclusions

- `drimmR`: drifting Markov models, reliability, different types of data.
- `smmR`: semi-Markov models, reliability, different types of sojourn time, censoring, non-parametric and parametric.
- `dsmmR`: drifting semi-Markov models, models 1, 2 and 3, non-parametric and parametric.

Future directions

- `hsmmR`: hidden semi-Markov models, reliability, different types of sojourn time, censoring, non-parametric and parametric (thanks to ANR HSMM-INCA).
- `gdrimmR`: generalized drifting Markov models, reliability (thanks to CNRS for E. Kalligeris contract).
- **Eye-Tracking**: work in collaboration with CETAPS to analyse climbing data. Clustering of models.