ZeSt Kolloquium

Mitigating consequences of the Markov property

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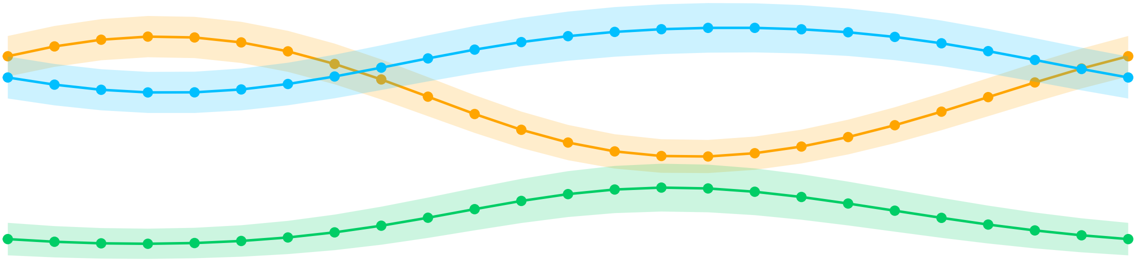
October 24, 2023



Outline

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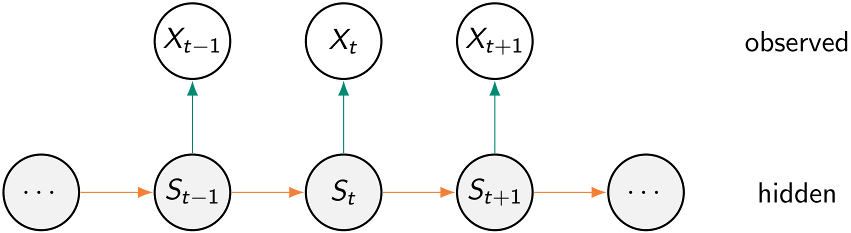
Quick Recap on HMMs

Doubly stochastic process:



- every observation is generated by one of N possible distributions $f_1, \ldots, f_N$,
- the state process selects which distribution is active at any given time point
- the state process is a **Markov chain**

Reminder: Markov chains

A Markov chain is a sequence of random variables $S_1, S_2, \dots$ that takes values in the *state space* $\{1, \dots, N\}$ and fulfills the *Markov property*

$$\Pr(S_{t+1} = s_{t+1} \mid S_1 = s_1, \dots, S_t = s_t) = \Pr(S_{t+1} = s_{t+1} \mid S_t = s_t).$$

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Due to this, we can characterise the state process by specifying the **initial distribution**

$$\boldsymbol{\delta}^{(1)} = (\Pr(S_1 = 1), \dots, \Pr(S_1 = N))$$

and the **transition probabilities**

$$\gamma_{ij}^{(t)} = \Pr(S_{t+1} = j \mid S_t = i).$$

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We summarise the transition probabilities in the **transition probability matrix** (t.p.m.)

$$\boldsymbol{\Gamma}^{(t)} = (\gamma_{ij}^{(t)})_{i,j=1,\dots,N}.$$

Why deal with the Markov property?

The Markov property and state dwell-times

In a homogeneous Markov chain, leaving a state can be interpreted as a repeated Bernoulli trial

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$$\begin{aligned}
\Pr(R=1) &= 1-\gamma_{11} \\
\Pr(R=2) &= \gamma_{11}\,(1-\gamma_{11}) \\
&\ldots \\
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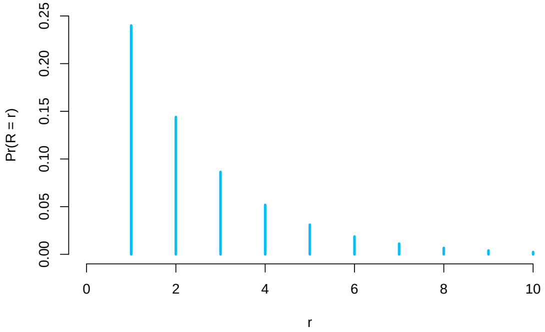
$$\dots$$
$$\Pr(R=r) = \gamma_{11}^{r-1}(1-\gamma_{11})$$

$R \sim \text{Geom}(1-\gamma_{11})$



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The **Markov property** and **geometric** dwell times are two sides of the same coin: **Memorylessness** of the process

Motivation

1. How problematic is the Markov property in more complex models? (including periodic variation)

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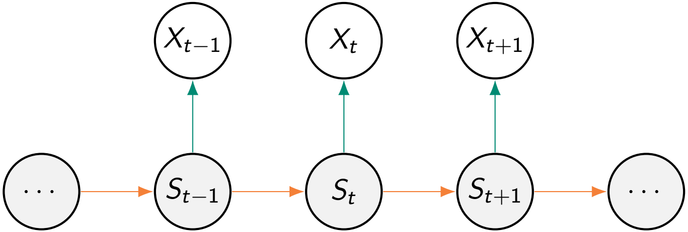
2. What about other options? (Hidden semi-Markov models)

Outline

Inhomogeneity in the state process



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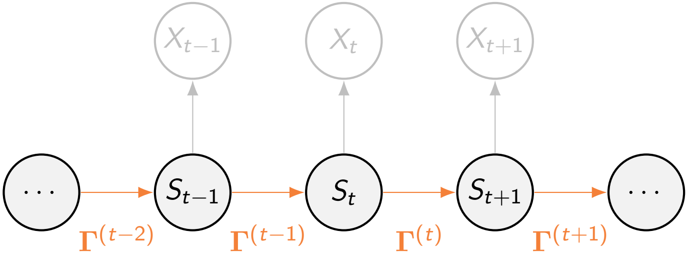

Periodic variation

Periodically varying transition probabilities formally means:

$$\mathbf{\Gamma}^{(t)} = \mathbf{\Gamma}^{(t+L)} \quad \text{for all } t = 1, \ldots, T, \tag{1}$$

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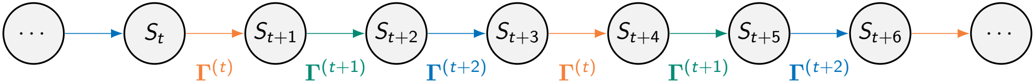

Recap: Stationarity

Homogeneous and "well-behaved"[1] Markov chains converge against their stationary distribution.

$$\Pr(S_t = i) \to \delta_i$$

where $\boldsymbol{\delta}$ is the solution to

$$\boldsymbol{\delta}\boldsymbol{\Gamma} = \boldsymbol{\delta}, \quad \text{s.t.} \sum_{i=1}^{N} \delta_i = 1.$$

δ_i is a useful summary statistic: Average time spent in state i.

[1]Finite state space, irreducible and aperiodic.

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- But this estimate is biased!

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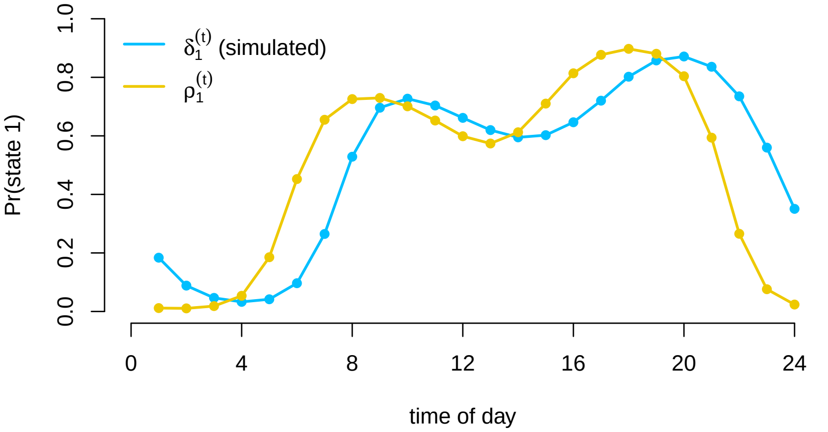

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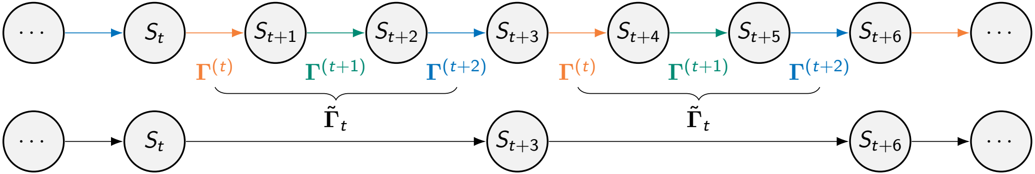

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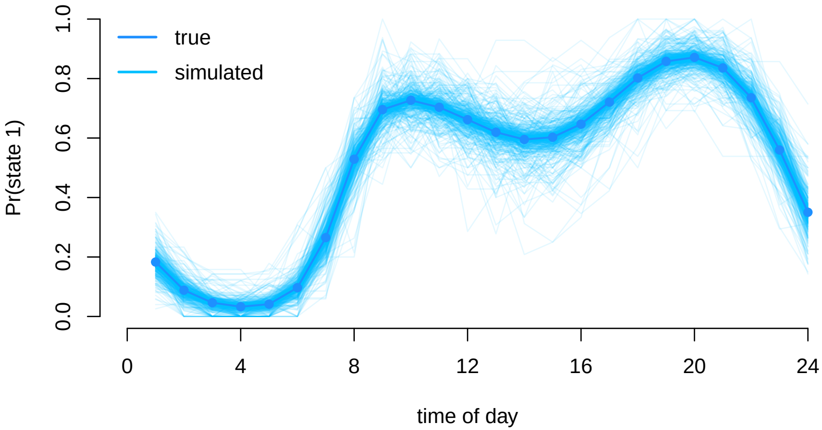
- It has constant t.p.m.

$$\tilde{\boldsymbol{\Gamma}}_t = \boldsymbol{\Gamma}^{(t)} \cdot \boldsymbol{\Gamma}^{(t+1)} \cdot \ldots \cdot \boldsymbol{\Gamma}^{(t+L-1)}.$$

- Thus each thinned chain converges, and we get $\Pr(S_t = i)$ for each t by solving

$$\boldsymbol{\delta}^{(t)} \tilde{\boldsymbol{\Gamma}}_t = \boldsymbol{\delta}^{(t)} \quad \text{s.t.} \sum_{i=1}^{N} \delta_i^{(t)} = 1.$$

Periodic stationarity



Time-varying dwell-time distribution

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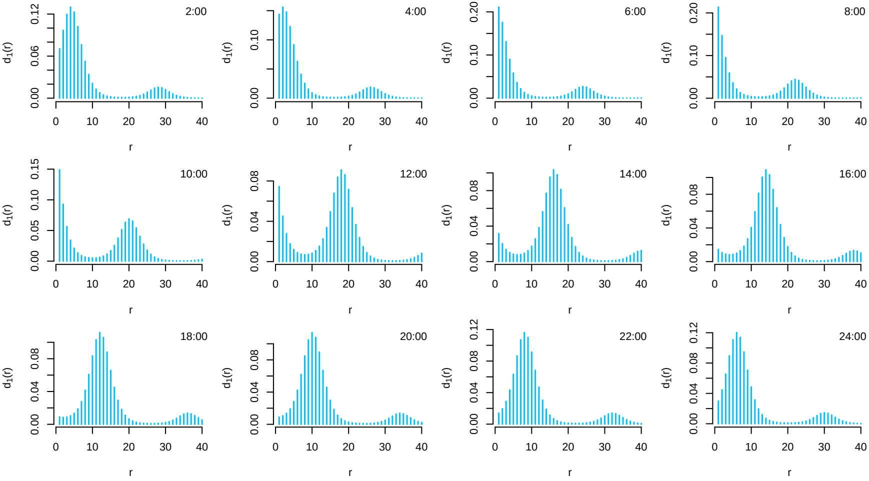
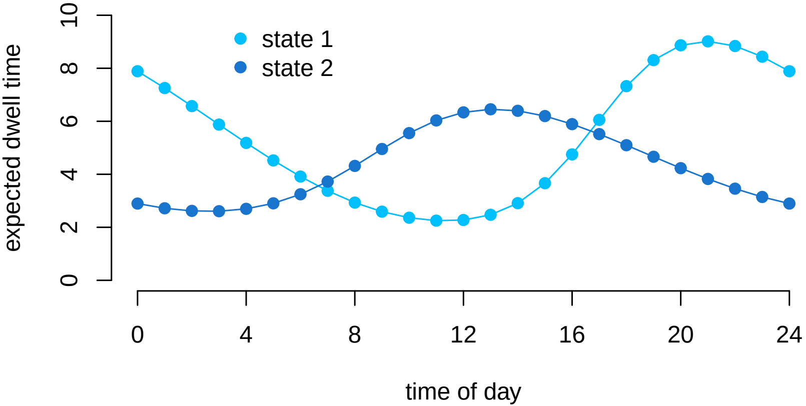
- To begin with, we can consider the dwell-time distribution at a certain time point:

$$d_i^{(t)}(r) = \underbrace{(1 - \gamma_{ii}^{(t+r-1)})}_{\text{leave}} \cdot \underbrace{\prod_{j=1}^{r-1} \gamma_{ii}^{(t+j-1)}}_{\text{stay r times}}, \qquad r \in \mathbb{N}$$

Time-varying dwell-time distribution



Expected (time-varying) dwell time



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- but we want something simpler for inference and model checking.
- We want to find the *overall* dwell-time distribution of a given state...

Overall dwell-time distribution

We can obtain the overall dwell-time distribution as a mixture:

$$d_i(r) = \sum_{t=1}^{L} w_i^{(t)} d_i^{(t)}(r), \qquad r \in \mathbb{N}$$

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$$d_i(r) = \sum_{t=1}^{L} w_i^{(t)} d_i^{(t)}(r), \qquad r \in \mathbb{N}$$

with the mixture weights defined as

$$w_i^{(t)} = \frac{\sum_{l \neq i} \delta_l^{(t-1)} \gamma_{li}^{(t-1)}}{\sum_{t=1}^{L} \sum_{l \neq i} \delta_l^{(t-1)} \gamma_{li}^{(t-1)}}, \qquad t = 1, \ldots, L,$$

where $\boldsymbol{\delta}^{(t)}$ is the periodically stationary distribution.

Overall dwell-time distribution

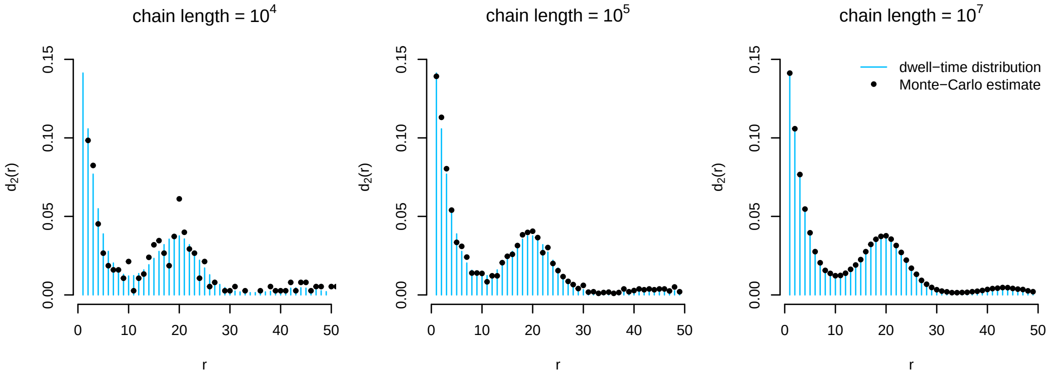
What we have here is

$$\frac{\sum_{t=1}^{L} \Pr(\text{Transition to state } i \text{ at time } t \text{ and stay } r \text{ times})}{\Pr(\text{Transition to state } i \text{ happens at some point of the day})}$$

$$= \frac{\Pr(\text{Transition to state } i \text{ and stay } r \text{ times at some point of the day})}{\Pr(\text{Transition to state } i \text{ happens at some point of the day})}$$

$$= \Pr(\text{Stay } r \text{ times in state } i \mid \text{Transition to } i \text{ happens at some point of the day})$$

Overall dwell-time distribution



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Concluding remarks:

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- But this may be limited to scenarios with a large amount of periodic variation.
- Thus, we need even more flexible models...

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Hidden semi-Markov models

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- But estimation and inference become more involved ...

Constructing a semi-Markov chain

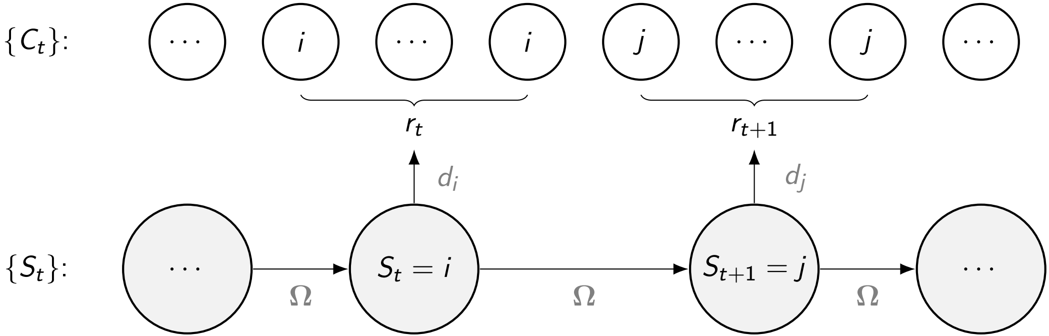
Instead of just a t.p.m., we need two ingredients:

- A set of dwell-time distributions $d_1, d_2, \dots, d_N$ with support $\mathbb{N}$ that determine the time-spent in a state.
- The conditional transition probabilities

$$\omega_{ij} = \Pr(S_{t+1} = j \mid S_t = i, S_{t+1} \neq i), \quad i,j = 1, \dots, N, \quad i \neq j,$$

given that the current state is left.

Constructing a semi-Markov chain



Approximation of a semi-Markov chain (Toy example)

Say we want to approximate a 2-state semi-Markov chain with

- dwell time in state 1 $\sim$ shiftedPois(λ) $\rightarrow$ p.m.f.: $d(r)$
- dwell time in state 2 $\sim$ Geom($1 - \gamma$)

and conditional t.p.m.

$$\boldsymbol{\Omega} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

To approximate the dwell-time distribution in state 1, we replace it with a **state aggregate** of size 3.

Approximation of a semi-Markov chain

We build a new Markov chain with the following block t.p.m.

$$\boldsymbol{\Gamma} = \left(\begin{array}{ccc|c} 0 & 1-c(1) & 0 & c(1) \\ 0 & 0 & 1-c(2) & c(2) \\ 0 & 0 & 1-c(3) & c(3) \\ \hline 1-\gamma & 0 & 0 & \gamma \end{array}\right)$$

where

$$c(r) = \begin{cases} \frac{d(r)}{1-F(r-1)} & \text{for } F(r-1) < 1, \\ 1 & \text{for } F(r-1) = 1 \end{cases} \qquad (= \Pr(R = r \mid R \geq r))$$

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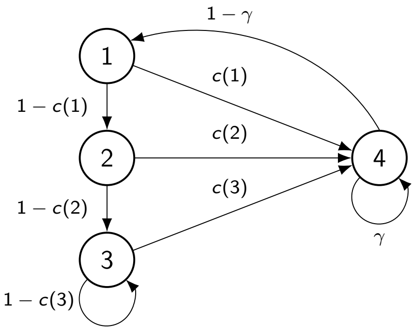
$$d^*(2) = (1 - c(1)) \cdot c(2) = (1 - d(1)) \cdot \frac{d(2)}{1 - d(1)} = d(2).$$

Approximation of a semi-Markov chain

- Paths through the state aggregate yield a **telescoping product** $\rightarrow$ Exact representation up to the chosen aggregate size.
- For dwell times larger than 3, so-called geometric tail:

$$d^*(r) = d(3) \cdot (1 - c(3))^{r-3}$$

Approximation of a semi-Markov chain



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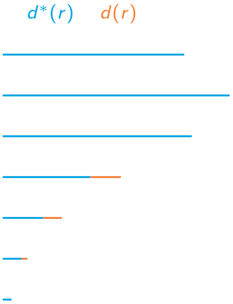
$$d^*(4) = d(3)(1 - c(3))$$

$$d^*(5) = d(3)(1 - c(3))^2$$

$$d^*(6) = d(3)(1 - c(3))^3$$

$$\ldots$$



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- In doing so we represent an HSMM by a regular HMM with an enlarged state space and structured transition probabilities.
- Parameter estimation via numerical maximum likelihood and standard inference.

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- Typically by linking the mean to external covariates, e.g. $d_i^{(t)} = \text{shiftedPois}(\lambda_i^{(t)})$ where $\lambda_i^{(t)} = \exp(\boldsymbol{\beta}_i' \boldsymbol{z}_t)$ for some set of external covariates $\boldsymbol{z}_t$, $t = 1, \ldots, T$.

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- The conditional transition probabilities $\omega_{ij}^{(t)}$ may also be inhomogeneous, but we will ignore that for now (well explored).

Here comes the tricky part

- We will do the same as before (but now with general notation) **and** add the inhomogeneity.
- Now for $i = 1, \ldots, N$ consider the inhomogeneous hazard rates

$$c_i^{(t)}(r) = \begin{cases} \frac{d_i^{(t)}(r)}{1 - F_i^{(t)}(r-1)} & \text{for } F_i^{(t)}(r-1) < 1, \\ 1 & \text{for } F_i^{(t)}(r-1) = 1 \end{cases}$$

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- For $t = 1, \dots, T$ consider the structured block t.p.m.

$$\boldsymbol{\Gamma}^{(t)} = \begin{pmatrix} \boldsymbol{\Gamma}_{11}^{(t)} & \cdots & \boldsymbol{\Gamma}_{1N}^{(t)} \\ \vdots & \ddots & \vdots \\ \boldsymbol{\Gamma}_{N1}^{(t)} & \cdots & \boldsymbol{\Gamma}_{NN}^{(t)} \end{pmatrix}$$

Inhomogeneous HSMMs

The diagonal block matrices ($N_i \times N_i$) are now inhomogeneous and are defined as

$$\mathbf{\Gamma}_{ii}^{(t)} = \begin{pmatrix} 0 & 1 - c_i^{(t)}(1) & 0 & \cdots & & 0 \\ 0 & 0 & 1 - c_i^{(t-1)}(2) & \cdots & & 0 \\ 0 & 0 & 0 & \ddots & & 0 \\ \vdots & \vdots & & & & \vdots \\ 0 & 0 & \cdots & & 0 & 1 - c_i^{(t-N_i+2)}(N_i - 1) \\ 0 & 0 & \cdots & & 0 & 1 - c_i^{(t-N_i+1)}(N_i) \end{pmatrix}.$$

Inhomogeneous HSMMs

The off-diagonal block matrices ($N_i \times N_j$) are defined as

$$\mathbf{\Gamma}_{ij}^{(t)} = \begin{pmatrix} \omega_{ij} c_i^{(t)}(1) & 0 & \cdots & 0 \\ \omega_{ij} c_i^{(t-1)}(2) & 0 & \cdots & 0 \\ \vdots & & & \\ \omega_{ij} c_i^{(t-N_i+1)}(N_i) & 0 & \cdots & 0 \end{pmatrix}.$$

Example

$$\Gamma_{ii}^{(t)} = \begin{pmatrix} 0 & \mathbf{1 - c_i^{(t)}(1)} & 0 & \cdots & 0 \\ 0 & 0 & 1 - c_i^{(t-1)}(2) & \cdots & 0 \\ 0 & 0 & 0 & \ddots & 0 \\ \vdots & \vdots & & & \vdots \end{pmatrix}$$

$$\Gamma_{ii}^{(t+1)} = \begin{pmatrix} 0 & 1 - c_i^{(t+1)}(1) & 0 & \cdots & 0 \\ 0 & 0 & \mathbf{1 - c_i^{(t)}(2)} & \cdots & 0 \\ 0 & 0 & 0 & \ddots & 0 \\ \vdots & \vdots & & & \vdots \end{pmatrix}$$

Example

$$\mathbf{\Gamma}_{ij}^{(t+2)} = \begin{pmatrix} \omega_{ij} c_i^{(t+2)}(1) & 0 & \cdots & 0 \\ \omega_{ij} c_i^{(t+1)}(2) & 0 & \cdots & 0 \\ \omega_{ij} \mathbf{c_i^{(t)}(3)} & 0 & \cdots & 0 \\ \vdots & & & \end{pmatrix}$$

The ω_{ij} are summed out by total probability.

Inhomogeneous HSMMs

- Dwell time in a state aggregate is again determined by the superdiagonal of $\mathbf{\Gamma}_{ii}^{(t)}$
- Due to the inhomogeneity path runs through $\mathbf{\Gamma}^{(t)}, \mathbf{\Gamma}^{(t+1)}, \mathbf{\Gamma}^{(t+2)}, \dots$
- The implemented time-shift renders the dwell-time distriution $d_i^{(t)}$ when the transition into that state aggregate happends in t.
- We have arrived at **fully inhomogeneous HSMMs**.[2]

[2] Covariates in the dwell-time distributions, conditional transition probabilities and the state-dependent process.

Dwell-time distribution of inhomogeneous HSMMs

- I already mentioned some advantages of approximating HSMMs with HMMs
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- Another very nice one: All theory established before applies very similarly when we restrict ourselves to periodic variation as a covariate.
- We can calculate the periodically stationary distributions,
- and the overall state dwell-time distribution...

Dwell-time distribution of inhomogeneous HSMMs

$$d_i(r) = \sum_{t=1}^{L} v_i^{(t)} d_i^{(t)}(r), \quad \text{for } r \leq N_i,$$

with the mixture weights defined as

$$v_i^{(t)} = \frac{\sum_{l \in I_k, k \neq i} \delta_l^{(t-1)} \gamma_{l I_i^-}^{(t-1)}}{\sum_{t=1}^{L} \sum_{l \in I_k, k \neq i} \delta_l^{(t-1)} \gamma_{l I_i^-}^{(t-1)}}, \quad t = 1, \ldots, L,$$

where I_i^- is the lowest state of state aggregate i and $\boldsymbol{\delta}^{(t)}$ is the stationary distribution at t.

Outline

Application: Drosophila melanogaster

Figure 1: Source: https://de.wikipedia.org/wiki/Drosophila_melanogaster.

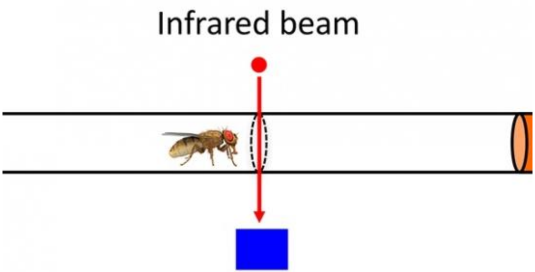

Figure 2: Source: https://www.eurekalert.org/multimedia/670792.

Application: Drosophila melanogaster

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- two conditions: Light-Dark (LD) and only Dark (DD)
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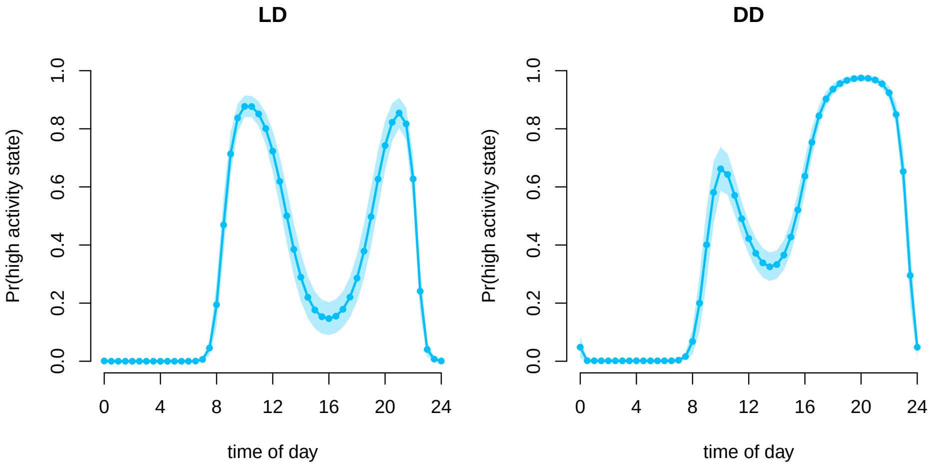
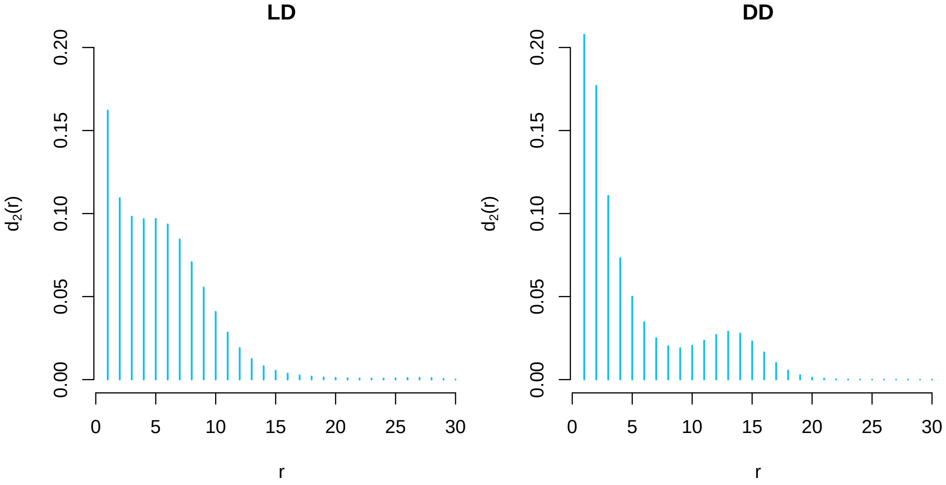
Application: Drosophila melanogaster



Application: Drosophila melanogaster



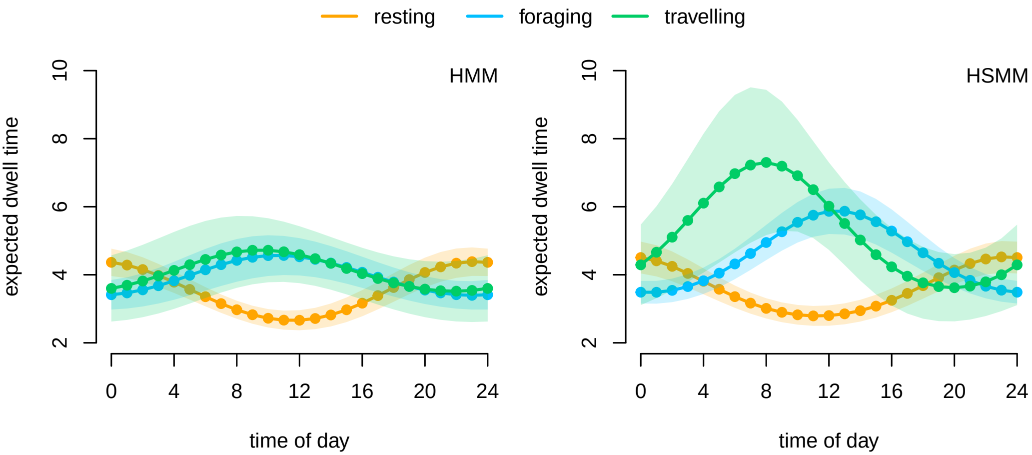
Application: Arctic muskox

Figure 3: Source: https://en.wikipedia.org/wiki/Muskox

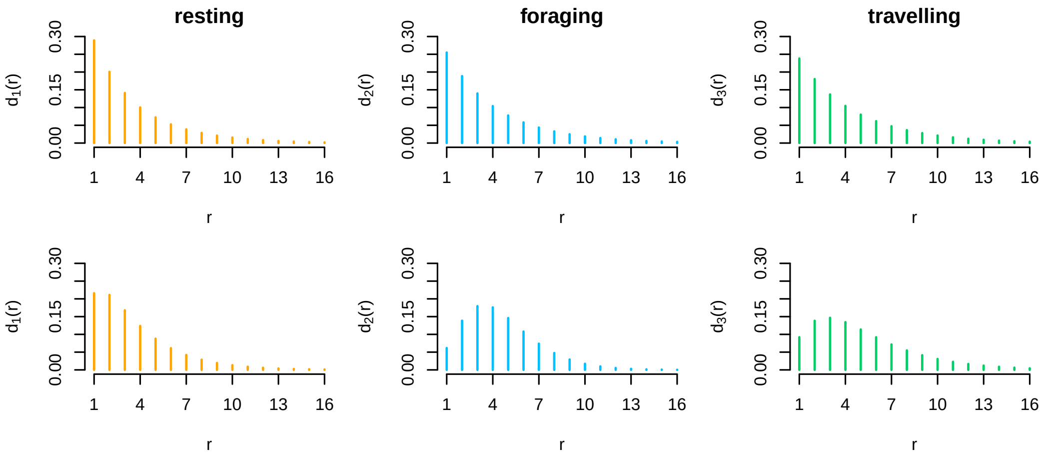
Application: Arctic muskox

- Largest arctic herbivore
- Previous analyses revealed non-geometric dwell times and temporal variation (Pohle, Langrock, et al., 2017; Beumer et al., 2020; Pohle, Adam, et al., 2022)
- 3-state HMMs and HSMMs: resting, foraging and travelling

Application: Arctic muskox



Overall dwell-time distributions



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Conclusion and Outlook

- Having a closer look at widely used HMMs with periodic variation enables us to conduct new inference.
- In periodic HMMs, dwell time can be very non-geometric
- Thus, criticising the Markov assumption by addressing geometric dwell-times falls short of such models' actual potential.
- Some scenarios still require flexible modelling of state dwell times that are not well described by periodic variation only.
- The muskox example showed that in scenarios with non-geometric dwell times and additional inhomogeneity, inhomogeneous HSMMs become worthwile.

Literature

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Thank you very much for your attention!