Bayesian Inference of Information Transfer in Networked Multi-Agent Systems

TECHNISCHE UNIVERSITÄT DARMSTADT

Master-Thesis

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Introduction

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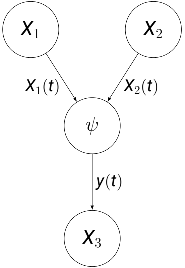
- Problem: Agent making decisions based on incoming messages, but observes only a summary of them
- Objective: To infer this observation model from agent's behaviour
- Motivation: Cell to cell communication and cellular decision making **[?]**
  - A cell may emit some message based on its gene activation state. Consider two cells emitting messages, a third cell receiving a translation of these messages. Third cell may have evolved to achieve some task in coordination with other cells.
    e.g. the messages containing information about consumption of a particular molecule which needs to be partitioned for survival.
- Assuming that the behaviour of agent has been shaped by evolution (close) to optimality



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Graphical Model

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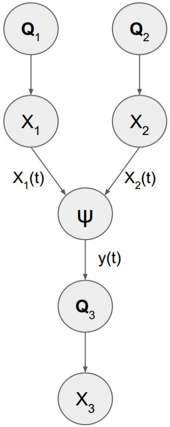


- X_1 and X_2 homogenous continuous-time Markov processes with $\mathbf{Q}_1$ and $\mathbf{Q}_2$ transition intensity matrices

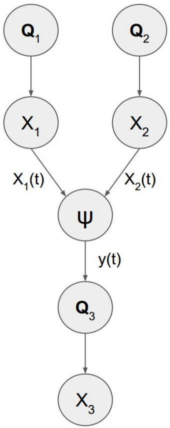
$$\mathbf{Q}_i \sim Gam(\alpha_i, \beta_i), \quad i \in \{1, 2\} \tag{1}$$

- X_3 inhomogeneous continuous-time Markov process with set of actions $a \in \{a_0, a_1\}$ and set of transition intensity matrices $\mathbf{Q}_3 = \{\mathbf{Q}_{a_0}, \mathbf{Q}_{a_1}\}$

$$\mathbf{Q}_a \sim Gam(\alpha_a, \beta_a) \tag{2}$$

- $\mathcal{X}_i = \{0, 1\}$
- $\psi := p(y(t) \mid X_1(t), X_2(t))$ observation model
- $b(x_1, x_2; t)$: belief state
- $\pi(a \mid b)$: optimal policy of X_3
- $X_i^{[0,T]}$: discrete valued trajectory in time interval $[0, T]$

Problem Statement



- While acting in the environment, the agent is assumed to have access to following parameters:
  - Transition intensity matrices of the parents $\mathbf{Q}_1$ and $\mathbf{Q}_2$
  - Observation model ψ
  - The optimal policy and $\boldsymbol{Q}_3$
- For the inference problem, the following parameters are given:
  - Transition intensity matrices of the parents $\mathbf{Q}_1$ and $\mathbf{Q}_2$
  - The optimal policy and $\boldsymbol{Q}_3$

Belief State $b(x_1, x_2; t)$

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- Belief state is the probability distribution over state space given the observations

$$b(x_1, x_2; t) = P(X_1(t) = x_1, X_2(t) = x_2 \mid y_1, ..., y_t) \tag{3}$$

- Denote $b(t)$, $t \geq 0$, as row vector with $\{b(x_1, x_2; t)_{x_i \in \mathcal{X}_i}\}$.
- This posterior probability can be described by a system of ODEs

$$\frac{db(t)}{dt} = b(t)\,\mathbf{T} \tag{4}$$

where the initial condition $b(0)$ is row vector with $\{P(X_1(0) = x_1, X_2(0) = x_2)_{x_i \in \mathcal{X}_i}\}$ **[?]**.

- $\mathbf{T}$ is the joint transition intensity matrix of X_1 and X_2 and given by amalgamation operation between $\mathbf{Q}_1$ and $\mathbf{Q}_2$ **[?]**.

$$\mathbf{T} = \mathbf{Q}_1 * \mathbf{Q}_2 \tag{5}$$

Belief Update

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- The belief update at discrete times of observation y_t

$$
\begin{aligned}
b(x_1, x_2; t) &= P(X_1(t) = x_1, X_2(t) = x_2 \mid y_1, \ldots, y_t) \\
&= \frac{P(y_1, \ldots, y_t, X_1(t) = x_1, X_2(t) = x_2)}{P(y_1, \ldots, y_t)} \\
&= \frac{P(y_t \mid y_1, \ldots, y_{t-1}, X_1(t) = x_1, X_2(t) = x_2)}{P(y_t \mid y_1, \ldots, y_{t-1})} \frac{P(y_1, \ldots, y_{t-1}, X_1(t) = x_1, X_2(t) = x_2)}{P(y_1, \ldots, y_{t-1})} \\
&= Z_t^{-1} \, P(y_t \mid x_1, x_2) \, P(X_1(t) = x_1, X_2(t) = x_2 \mid y_1, \ldots, y_{t-1}) \\
&= Z_t^{-1} \, {\color{blue} P(y_t \mid x_1, x_2)} \, {\color{red} b(x_1, x_2; t^-)}
\end{aligned} \tag{6}
$$

where $Z_t = \sum_{x_1, x_2 \in X} P(y_t \mid x_1, x_2) \, b(x_1, x_2; t^-)$ is the normalization factor **[?]**.

Inhomogeneous Transition Intensity Matrix $\mathbf{Q}_3(t)$

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- Let $\pi(a \mid b)$ be an optimal policy, where $a \in \{a_0, a_1\}$ is action, and $\boldsymbol{Q}_3 = \{\mathbf{Q}_{a_0}, \mathbf{Q}_{a_1}\}$ be a set of intensity matrices of X_3 corresponding to each action.
- The inhomogeneous transition intensity matrix $\mathbf{Q}_3(t)$ can be written as

$$\mathbf{Q}_3(t) = \sum_a \mathbf{Q}_a \, \pi(a \mid b(x_1, x_2; t)). \tag{7}$$

Markov Processes

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- Consider a homogenous Markov process X with values $\mathcal{X} = \{x_0, x_1, ..., x_n\}$. The transition intensity matrix **Q** of such process has the following form:

$$\mathbf{Q} = \begin{bmatrix} -q_{x_0} & q_{x_0 x_1} & \cdots & q_{x_0 x_n} \\ q_{x_1 x_0} & -q_{x_1} & \cdots & q_{x_1 x_n} \\ \vdots & \vdots & \ddots & \cdots \\ q_{x_n x_0} & q_{x_n x_1} & \cdots & -q_{x_n} \end{bmatrix} \tag{8}$$

  where $q_x = \sum_{x' \neq x, x' \in \mathcal{X}} q_{xx'}$.
- The amount of time that X stays in a transitioned state is exponentially distributed, and the probability density function of staying in a state x is given by **[?]**

$$f(t) = q_x \, exp(-q_x t). \tag{9}$$

Likelihood Functions

Homogenous continuous-time Markov process

- The likelihood of a single transition $d = \langle x, t, x' \rangle$, where transition happens from x to x' after spending time amount of time t:

$$P(d \mid \mathbf{Q}) = (q_x \, exp(-q_x t)) \left(\frac{q_{xx'}}{q_x} \right) \tag{10}$$

- The likelihood of trajectory $X^{[0,T]}$ can be decomposed as a product of likelihood of single transitions.

$$\begin{aligned} P(X^{[0,T]} \mid \mathbf{Q}) &= \left(\prod_x q_x^{M[x]} \, exp(-q_x T[x]) \right) \left(\prod_x \prod_{x' \neq x} \frac{q_{xx'}}{q_x}^{M[x,x']} \right) \\ &= \prod_x exp(-q_x T[x]) \prod_{x' \neq x} q_{xx'}^{M[x,x']} \end{aligned} \tag{11}$$

where $T[x]$ is the total time spent in state x, $M[x, x']$ is the number of transitions from state x to state x', $M[x]$ is total number of transitions leaving state x **[?]**.

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- Similarly, let X be an inhomogeneous Markov process, and **Q**(t) be the transition intensity matrix. The probability density function of staying in a state x is

$$f(t) = q_x(t)\ \exp\left(-\int q_x(u)du\right) \tag{12}$$

- The likelihood of trajectory $X^{[0,T]}$ with m transitions at $t_0, t_1, ..., t_m$ **[?]**

$$\begin{aligned} P(X^{[0,T]} \mid \mathbf{Q}^{[0,T]}) &= \prod_{k=1}^{m} \left[q_{x_{k-1}}(t_k) \exp\left(-\int_{t_{k-1}}^{t_k} q_{x_{k-1}}(u)du\right) \frac{q_{x_{k-1},x_k}(t_k)}{q_{x_{k-1}}(t_k)} \right] \\ &= \prod_{k=1}^{m} \left[q_{x_{k-1},x_k}(t_k)\ \exp\left(-\int_{t_{k-1}}^{t_k} q_{x_{k-1}}(u)du\right)\right]. \end{aligned} \tag{13}$$

Likelihood Model of the System

- Let D be a sample of trajectories in the dataset, such that $D = \left\langle X_1^{[0,T]}, X_2^{[0,T]}, X_3^{[0,T]} \right\rangle$, and the set of parameters to the system $\theta = \langle \mathbf{Q}_1, \mathbf{Q}_2, \mathbf{Q}_3, \pi, \psi \rangle$.
- The likelihood of the sample trajectory D can be written as

$$\begin{aligned} P(D \mid \theta) &= P(X_1^{[0,T]}, X_2^{[0,T]}, X_3^{[0,T]} \mid \mathbf{Q}_1, \mathbf{Q}_2, \mathbf{Q}_3, \pi, \psi) \\ &= P(X_3^{[0,T]} \mid X_1^{[0,T]}, X_2^{[0,T]}, \mathbf{Q}_1, \mathbf{Q}_2, \mathbf{Q}_3, \pi, \psi)\, P(X_1^{[0,T]} \mid \mathbf{Q}_1)\, P(X_2^{[0,T]} \mid \mathbf{Q}_2) \\ &= P(X_3^{[0,T]} \mid \mathbf{Q}_3^{[0,T]})\, P(X_1^{[0,T]} \mid \mathbf{Q}_1)\, P(X_2^{[0,T]} \mid \mathbf{Q}_2) \end{aligned} \tag{14}$$

where $\mathbf{Q}_3^{[0,T]}$ is a deterministic function of $X_1^{[0,T]}, X_2^{[0,T]}, \mathbf{Q}_1, \mathbf{Q}_2, \mathbf{Q}_3, \pi$ and ψ, given by Eq.7.

Simulation and Results
Parameters

- Intensity matrices

$$\mathbf{Q}_1 = \begin{bmatrix} -3.2 & 3.2 \\ 0.5 & -0.5 \end{bmatrix}$$

$$\mathbf{Q}_2 = \begin{bmatrix} -1.5 & 1.5 \\ 3.45 & -3.45 \end{bmatrix}$$

$$\mathbf{Q}_3 = \left\{ \begin{bmatrix} -0.5 & 0.5 \\ 25 & 25 \end{bmatrix}, \begin{bmatrix} -32 & 32 \\ 0.02 & -0.02 \end{bmatrix} \right\}$$

- Observation models

$$\psi_0 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

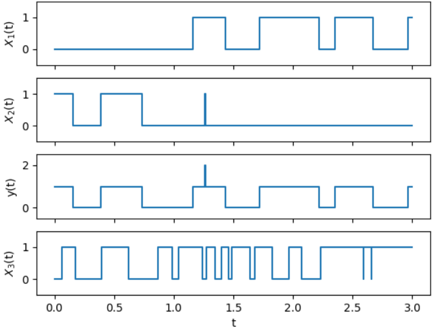
$$\psi_1 = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

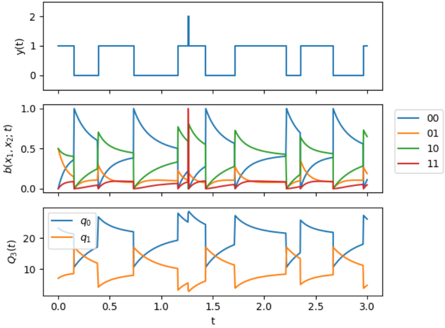
$$\psi_2 = \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}$$

Simulation

Sampling trajectories using Gillespie algorithm

- Sampled trajectory example:





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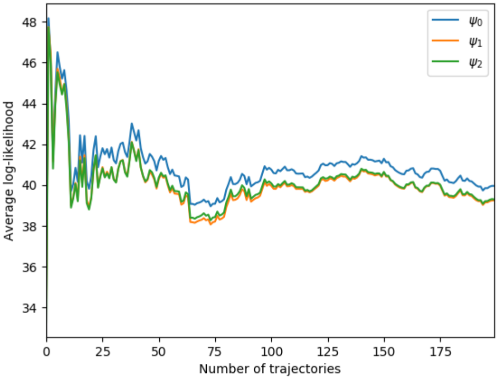
Results

Maximum likelihood estimation



- Observation models

$$\psi_0 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$\psi_1 = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$\psi_2 = \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}$$

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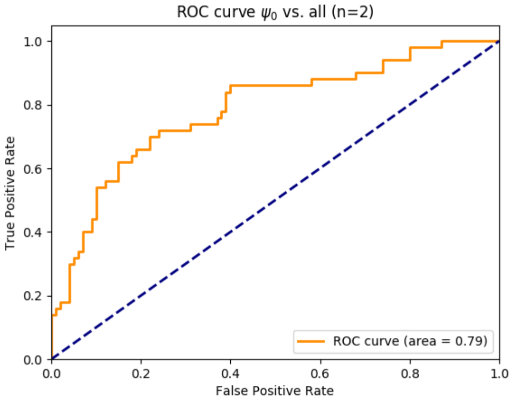
Results

Receiver Operating Characteristic(ROC) Analysis



- Classification problem between same observation models
- 300 trajectories, class-balanced

Conditional Intensity Marginalization

over $\mathbf{Q}_1$ and $\mathbf{Q}_2$

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- Replacing the exact belief update with marginal particle filter approximation
  - Removing the assumption that transition intensity matrices of X_1 and X_2 are available to agent X_3
  - More realistic system
- Given the priors and sample trajectory, the intensity matrices can be replaced by estimates. **[?]**
  - $\mathbf{Q}_i$ with non-diagonal entries $q^i_{xx'} \sim Gam(\alpha_i(x,x'), \beta_i(x,x')),\ \ i \in \{1,2\}$
  - $X_i^{[0,T]}$ with summary statistics $T_i[x]$ and $M_i[x,x']$, where $T_i[x]$ is the total time spent in state x, $M_i[x,x']$ is the number of transitions from state x to state x'
  - Using Bayes' rule and the likelihood of trajectory in Eq.11, the estimates can be evaluated analytically as follows:

$$E\left[q^i_{xx'} | X^{[0,T]}\right] = \frac{\alpha_i(x,x') + M_i[x,x']}{\beta_i(x,x') + T_i[x]} \tag{15}$$

Marginal Particle Filter

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- Given a prior distribution over states, the particles are initialized $\mathbf{p}^0$.

Algorithm 1: Marginal particle filter[?]

Input: Measurement data y_k at time t_k, set of particles $\mathbf{p}^{k-1}$
Result: New set of particles $\mathbf{p}^k$, representing $b(t_k)$

for $p_m \in \mathbf{p}^{k-1}$ **do**
    $p_m = \{x_m, \mathbf{T}_m, \mathbf{M}_m\} \leftarrow$ *Propagate particle through marginal process model from* t_{k-1} *to* t_k
    $w_m \leftarrow p(y_k \mid X(t_k) = x_m)$ `// observation likelihood`
end for
$w_m \leftarrow \frac{w_m}{\sum_m w_m}$ `// normalize weights`
for $p_m \in \mathbf{p}_k$ **do**
    $p_m \leftarrow$ *Sample from* p_k *with probabilities* w_m *with replacement*
end for

Future work

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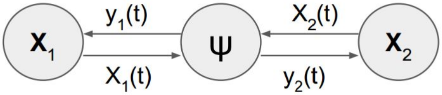
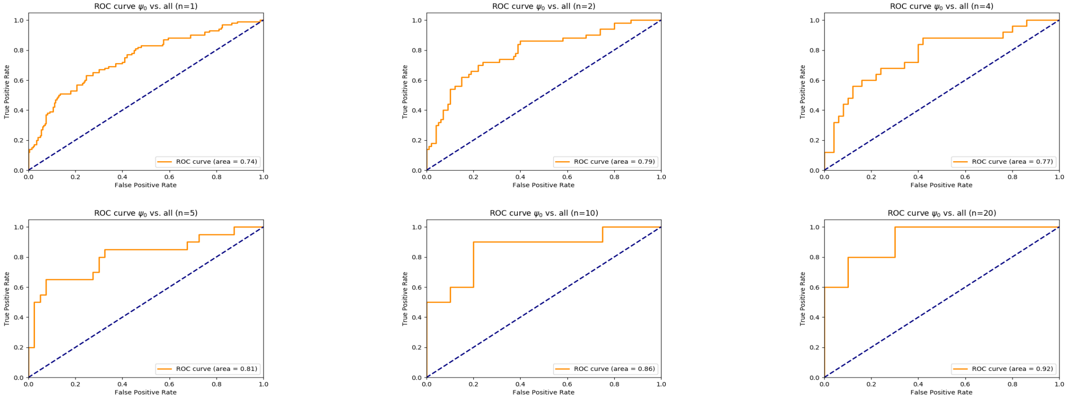
- Implementation of marginal particle filter
- Application on real-world data
  - e.g. British Household Panel Survey
- Inference of observation model in an interactive multi-agent system



References

Thank you!

Backup
ROC Analysis



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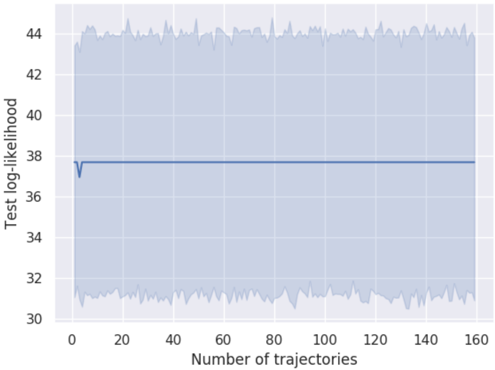
Backup
MLE



Test log-likelihood
30
32
34
36
38
40
42
44
0
20
40
60
80
100
120
140
160
Number of trajectories