# Learning interaction rules from multi-animal trajectories via augmented behavioral models


**Keisuke Fujii***
Nagoya University
RIKEN Center for Advanced Intelligence Project
JST PRESTO

**Naoya Takeishi**
University of Applied Sciences and Arts Western Switzerland
RIKEN Center for Advanced Intelligence Project

**Kazushi Tsutsui**
Nagoya University

**Emyo Fujioka**
Doshisha University

**Nozomi Nishiumi**
National Institute for Basic Biology

**Ryoya Tanaka**
Nagoya University

**Mika Fukushiro**
Doshisha University

**Kaoru Ide**
Doshisha University

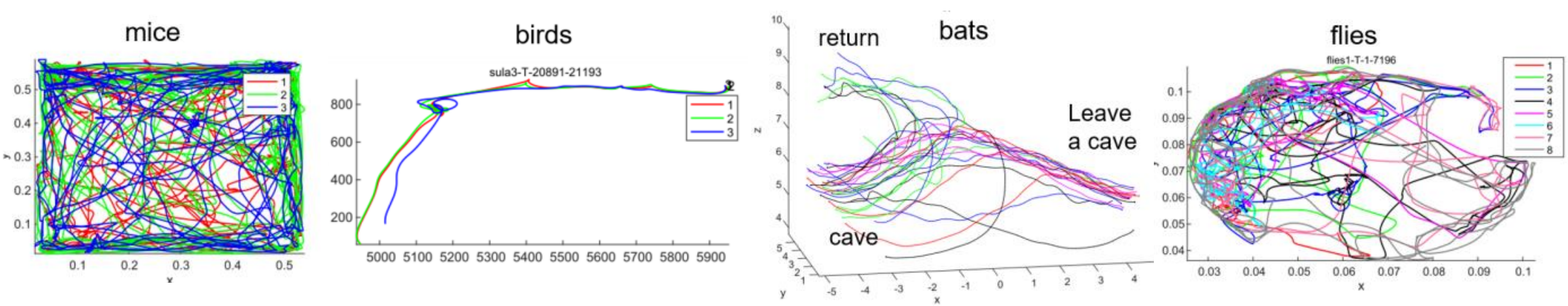
**Hiroyoshi Kohno**
Tokai University

**Ken Yoda**
Nagoya University

**Susumu Takahashi**
Doshisha University

**Shizuko Hiryu**
Doshisha University

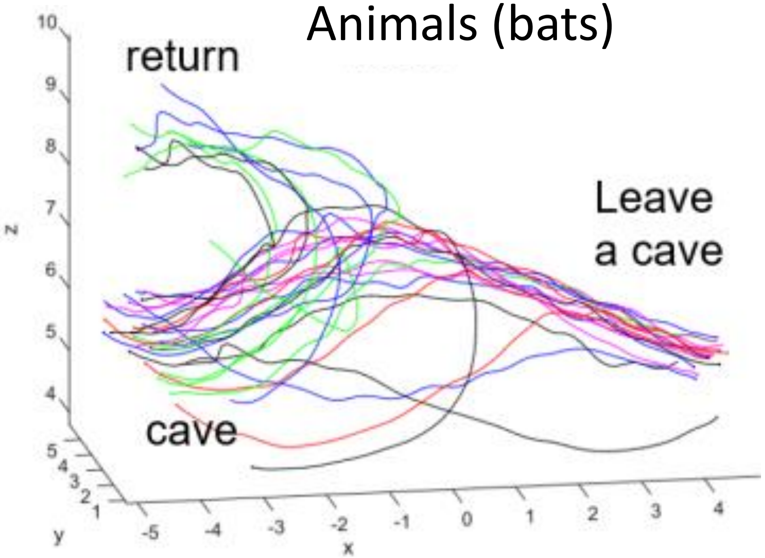
**Yoshinobu Kawahara**
Kyushu University
RIKEN Center for Advanced Intelligence Project

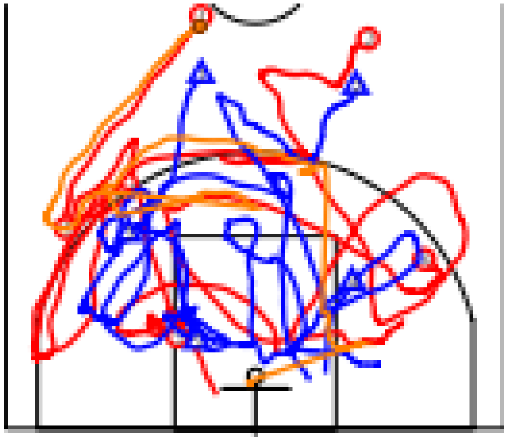
# Multi-agent movement sequences

Extracting the interaction rules of biological agents from movement sequences pose challenges in various domains

Animals (bats)




Humans (in basketball)



Other: pedestrians, vehicles .....

Discovering the directed interaction will contribute to the understanding of the principles of biological agents' behaviors

# Granger causality (GC) and problems

Granger causality [Granger, 1969] is a practical framework for exploratory analysis in various fields

- Recently: inferring GC under nonlinear dynamics [Tank+18; Khanna+19]

**Problem**: the structure of the generative process in biological multi-agent trajectories, which include time-varying dynamical systems, is not fully utilized in existing base models of GC (e.g., VAR and NN)

1. Ignoring the structures of such processes will lead to interpretational problems and sometimes erroneous assessments of causality

**solution**: incorporating the structures into the base model for inferring GC, e.g., augmenting (inherently) incomplete behavioral models with interpretable data-driven models, can solve these problems

2. Data-driven models sometimes detect false causality that is counterintuitive to the user of the analysis

**solution**: introducing architectures and regularization to utilize scientific knowledge will be effective for a reliable base model of a GC method

# Overview of our method

1. Formulation of augmented behavioral model (ABM) (sec. 3.2)

2. Learning of ABM (sec. 4.1)

3. Theory-guided regularization (sec. 4.2)

4. Inference of Granger causality (sec. 4.3)

(sec. is the reference to our paper)

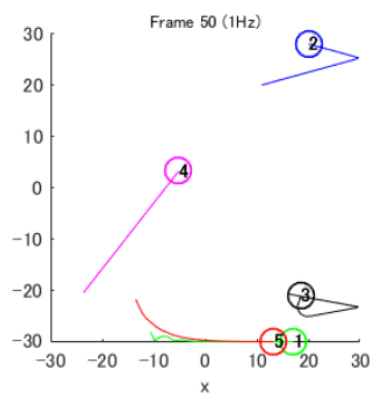
Conceptual animal behavioral model

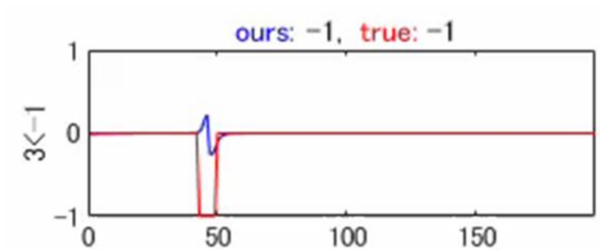
$$\boldsymbol{x}_{t+1}^{i} = f_{U}^{i}(f_{N}^{i}(\boldsymbol{r}_{t}^{i}, \boldsymbol{x}_{t}^{i}), f_{M}^{i}(\boldsymbol{r}_{t}^{i}, \boldsymbol{x}_{t}^{i}), \boldsymbol{r}_{t}^{i}, \boldsymbol{x}_{t}^{i})$$

Learning of ABM with NN

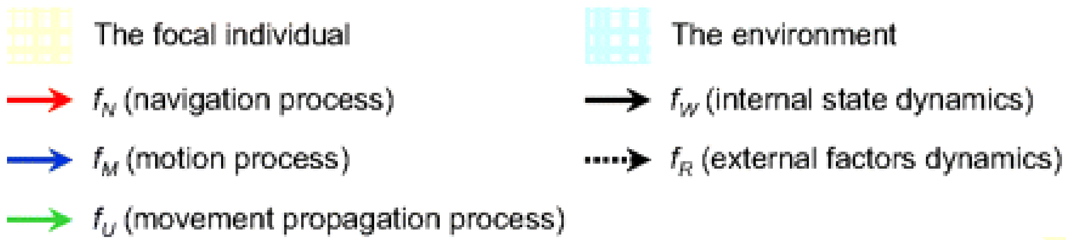
$$\boldsymbol{x}_{t}^{i} = \sum_{k=1}^{K} \left( F_{N}^{i,t,k}(\boldsymbol{h}_{t-k}^{i}) \odot F_{M}^{i,t,k}(\boldsymbol{h}_{t-k}^{i}) \right) \boldsymbol{h}_{t-k}^{i}$$

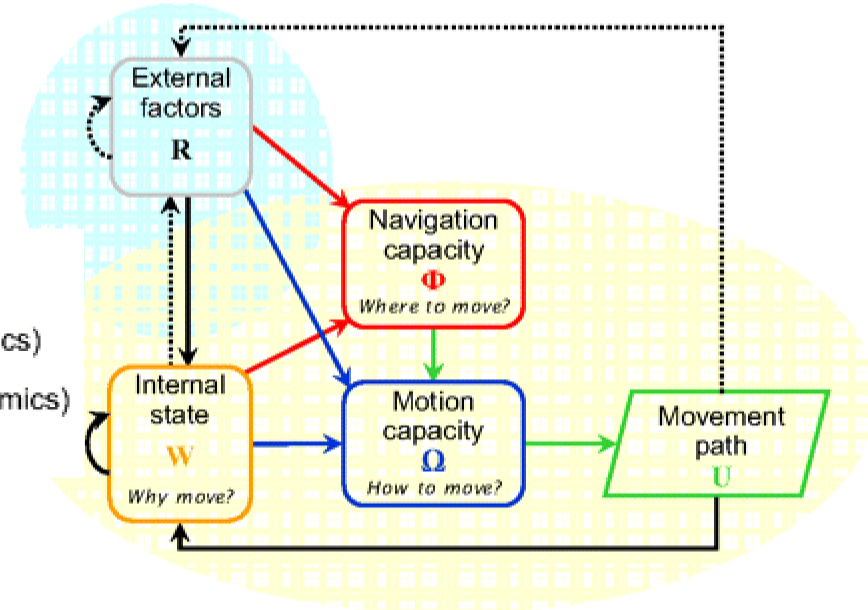
inferring time-varying GC



# 1. Formulation of ABM




[Nathan et al. PNAS, 2008]

Conceptual animal behavioral model (not numerically computable)

$$\boldsymbol{x}_{t+1}^i = f_U^i(f_N^i(\boldsymbol{r}_t^i, \boldsymbol{x}_t^i), f_M^i(\boldsymbol{r}_t^i, \boldsymbol{x}_t^i), \boldsymbol{r}_t^i, \boldsymbol{x}_t^i) + \boldsymbol{\varepsilon}_t^i$$

concatenated

Augmented Behavioral model (computable and interpretable)

$$\boldsymbol{x}_t^i = \sum_{k=1}^{K} \left( F_N^{i,t,k}(\boldsymbol{h}_{t-k}^i) \odot F_M^{i,t,k}(\boldsymbol{h}_{t-k}^i) \right) \boldsymbol{h}_{t-k}^i + \boldsymbol{\varepsilon}_t^i$$

Sign of GC (navigation) e.g., attraction and repulsion

positive weights of GC (motion)

It is closely related to self-explanatory NN [Alvarez-Melis & Jaakkola, 18] (sec. 3.3)

# 2. Learning of ABM

Learn $\Psi^i_{\theta_{t,k}}$ using MLP

$$x^i_t = \sum_{k=1}^{K} \Psi^i_{\theta_{t,k}} h^i_{t-k} + \varepsilon^i_t$$

where $$\Psi^i_{\theta_{t,k}} = \left( F_N^{i,t,k}(h^i_{t-k}) \odot F_M^{i,t,k}(h^i_{t-k}) \right)$$

Loss function

$$\sum_{t=K+1}^{T} \left( \mathcal{L}_{pred}(\hat{x}_t, x_t) + \lambda \mathcal{L}_{sparsity}(\Psi_t) + \gamma \mathcal{L}_{TG}(\Psi_t, \Psi_t^{TG}) \right) + \sum_{t=K+1}^{T-1} \beta \mathcal{L}_{smooth}(\Psi_{t+1}, \Psi_t)$$

(i) prediction loss

(ii) sparsity-inducing penalty term

(iii) theory-guided regularization term

(iv) smoothing penalty term

Concatenated weight matrix

$$[\Psi^1_{\theta_{t,K}}, \ldots, \Psi^1_{\theta_{t,1}}], \ldots, [\Psi^p_{\theta_{t,K}}, \ldots, \Psi^p_{\theta_{t,1}}]$$

Theory-guided weight (given in the next slide)

# 3. Theory-guided regularization

We estimate reliable GC by regularization using known scientific knowledge [Karpatne+ 17] (mainly studied on physical principles)

- Our basic idea: we utilize theory-based and data-driven prediction results and impose penalties in the appropriate situations

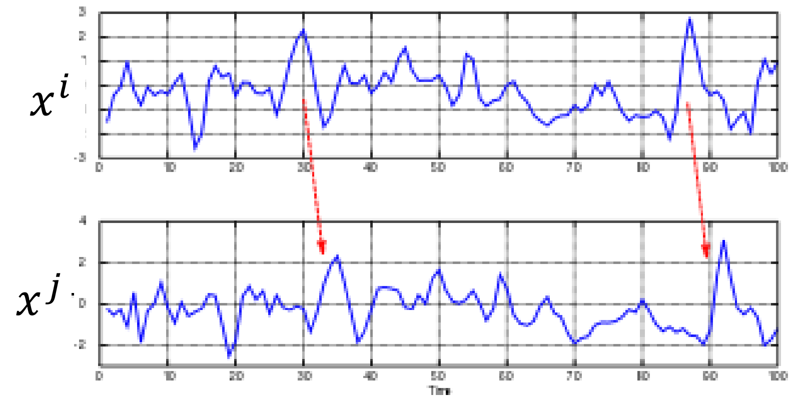
1. let $\widehat{\boldsymbol{x}}_t$ be the prediction from the data
2. prepare some input-output pairs（$\widetilde{\boldsymbol{x}}_{t-k\leq t}, \widetilde{\boldsymbol{x}}_t$）based on scientific knowledge
   - assume that the weight $\boldsymbol{\Psi}_t^{TG}$ is uniquely determined
   - this assumption reduces the possible pairs（$\widetilde{\boldsymbol{x}}_{t-k\leq t}, \widetilde{\boldsymbol{x}}_t$）
3. When $\widehat{\boldsymbol{x}}_t$ and $\widetilde{\boldsymbol{x}}_t$ are similar, impose penalties on the weights such that the cause of $\widehat{\boldsymbol{x}}_t$ (i.e., $\boldsymbol{\Psi}_t$) is similar to the cause of $\widetilde{\boldsymbol{x}}_t$ (i.e., $\boldsymbol{\Psi}_t^{TG}$).
   - we assume that the cause of $\widehat{\boldsymbol{x}}_t$ is equivalent to the cause of $\widetilde{\boldsymbol{x}}_t$ at the time

Here we utilize the only intuitive prior knowledge such that the agents go straight from the current state if there are no interactions

# 4. Inference of Granger Causality

## Recent definition of GC [Tank+18]:

A variable $x^i$ does not Granger-cause variable $x^j$, denoted as $x^i \nrightarrow x^j$, if and only if the prediction model of $x^j$ is constant in $x^i_{\leq t}$ .




(Wikipedia)

We here consider GC using the obtained $\mathbf{\Psi}_{i,j,t} \in \mathbb{R}^{K \times d \times d_r}$
In the following equation:

$d$: output dim.
$d_r$: input dim.
for each agent
(e.g., 2D or 3D)

$$S_{i,j,t} = \underset{1 \leq k \leq K}{\mathrm{signmax}} \left( \underset{\substack{q=1,\ldots,d_r \\ u=1,\ldots,d}}{\mathrm{median}} \left( \mathbf{\Psi}_{i,j,t} \right) \right) \max_{1 \leq k \leq K} \left( \| \left( \mathbf{\Psi}_{i,j} \right)_{t,k} \|_F \right)$$

signmax: sign of the larger value of max and min (e.g., signmax({1, 2, −3}) = −1)
$\| (\mathbf{\Psi}_{i,j})_{t,k} \|_F$ is the Frobenius norm of the matrix $(\mathbf{\Psi}_{i,j})_{t,k} \in \mathbb{R}^{d \times d_r}$

We consider $S_{i,j,t} \approx 0$ to be non-causal relationships and $S_{i,j,t} \gg 0$ if $x^i \rightarrow x^j$

# Experiments (1) Kuramoto model (synthetic data)

Kuramoto model
(nonlinear oscillators)

$$\frac{d\phi_i}{dt} = \omega_i + \sum_{j \neq i} k_{ij} \sin(\phi_i - \phi_j)$$

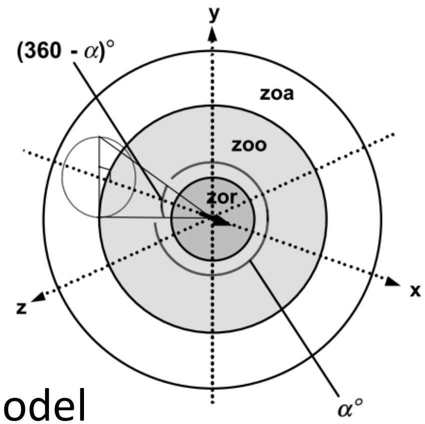
unknown causal relationship

## Experimental results

| | | Kuramoto model | | | |
|---|---|---|---|---|---|
| | | Acc. | Bal. Acc. | AUROC | AUPRC |
| | Linear GC | 0.655 ± 0.099 | 0.500 ± 0.000 | 0.546 ± 0.139 | 0.431 ± 0.143 |
| | Local TE | 0.335 ± 0.107 | 0.483 ± 0.050 | 0.489 ± 0.054 | 0.351 ± 0.104 |
| [Khanna+19] | eSRU [30] | 0.500 ± 0.092 | 0.500 ± 0.000 | 0.487 ± 0.123 | 0.548 ± 0.121 |
| [Löwe+20] | ACD [42] | 0.475 ± 0.121 | 0.528 ± 0.115 | 0.605 ± 0.135 | 0.519 ± 0.184 |
| [Marcinkevics+20] | GVAR [44] | 0.495 ± 0.154 | 0.473 ± 0.113 | 0.467 ± 0.079 | 0.398 ± 0.115 |
| w/o regularization | ABM - $\mathcal{L}_{TG}$ | **0.930± 0.075** | **0.914 ± 0.086** | **0.972 ± 0.036** | **0.929 ± 0.093** |
| | ABM (full) | 0.925 ± 0.075 | 0.902 ± 0.098 | **0.972 ± 0.036** | **0.929 ± 0.093** |

Although we used the dictionary of the functions with prior knowledge,
our method accurately detected the causality w/o theory-guided regularization

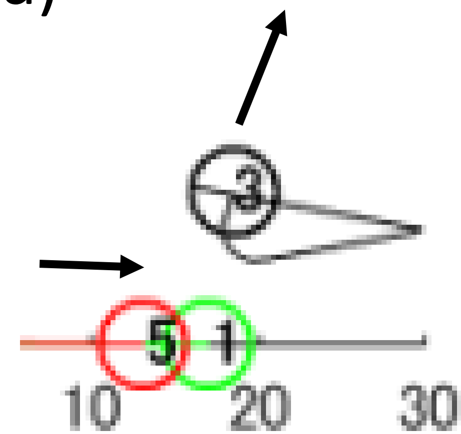
# Experiments (2) Boid model (synthetic data)




Boid model
[Couzin et al. 2002]

has only three rules: attraction, repulsion, and alignment

Here we set the boids directed preferences: true relations 1, 0, and −1 as attraction, no interaction, and repulsion

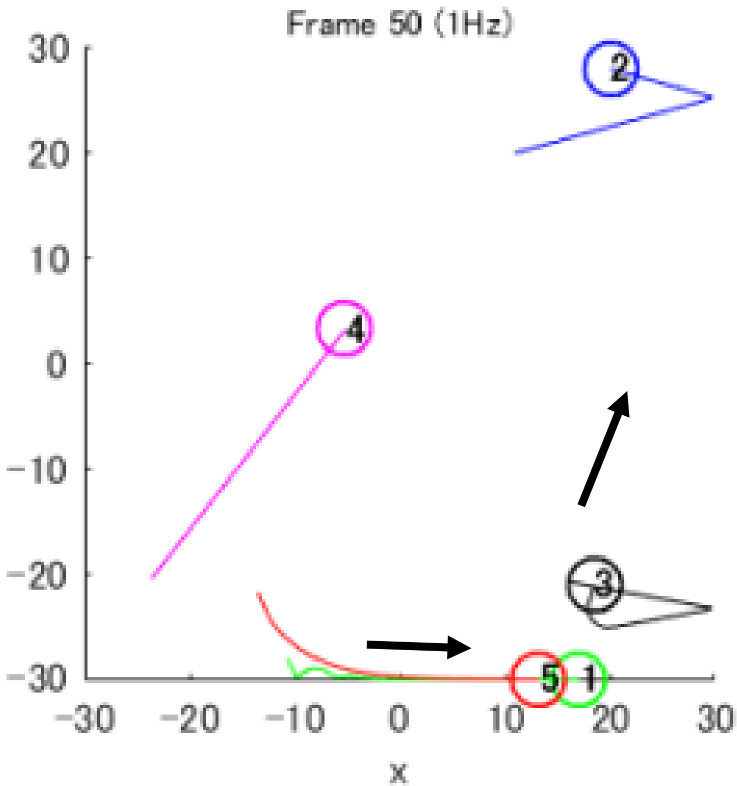


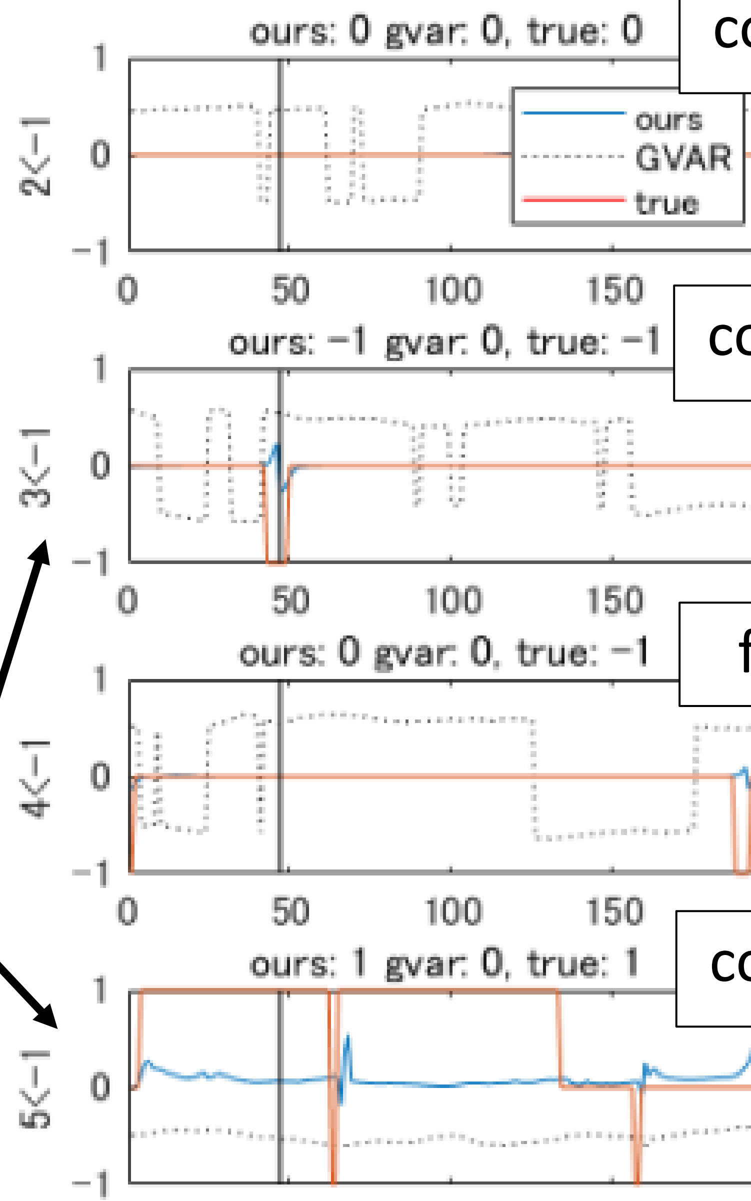

e.g., #1 attracts #5 (+1) and is avoid by #3 (-1)

## Experimental results: both learning of sign and TG regularization were needed

| | | Boid model | | | |
|---|---|---|---|---|---|
| | | Bal. Acc. | AUPRC | $BA_{pos}$ | $BA_{neg}$ |
| | Linear GC | 0.487 ± 0.028 | 0.591 ± 0.169 | 0.55 ± 0.150 | 0.530 ± 0.165 |
| | Local TE | 0.634 ± 0.130 | 0.580 ± 0.141 | N/A | N/A |
| [Khanna+19] | eSRU [30] | 0.500 ± 0.000 | 0.452 ± 0.166 | 0.495 ± 0.102 | 0.508 ± 0.153 |
| [Löwe+20] | ACD [42] | 0.411 ± 0.099 | 0.497 ± 0.199 | N/A | N/A |
| [Marcinkevics+20] | GVAR [44] | 0.441 ± 0.090 | 0.327 ± 0.119 | 0.524 ± 0.199 | 0.579 ± 0.126 |
| | ABM - $\boldsymbol{F}_N$ - $\mathcal{L}_{TG}$ | 0.500 ± 0.021 | 0.417 ± 0.115 | 0.513 ± 0.096 | 0.619 ± 0.157 |
| w/o learning of sign | ABM - $\boldsymbol{F}_N$ | 0.542 ± 0.063 | 0.385 ± 0.122 | 0.544 ± 0.160 | 0.508 ± 0.147 |
| w/o regularization | ABM - $\mathcal{L}_{TG}$ | 0.683 ± 0.124 | 0.638 ± 0.096 | 0.716 ± 0.172 | 0.700 ± 0.143 |
| | ABM (ours) | **0.767 ± 0.146** | **0.819 ± 0.126** | **0.724 ± 0.189** | **0.760 ± 0.160** |

# Experiments (2) an example of results in boid model




correct

correct

false

correct

e.g., #1 is avoid by #3 (-1)
and attracts #5 (+1)

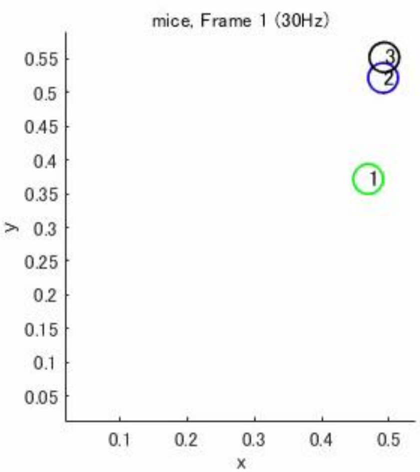
positive: attraction

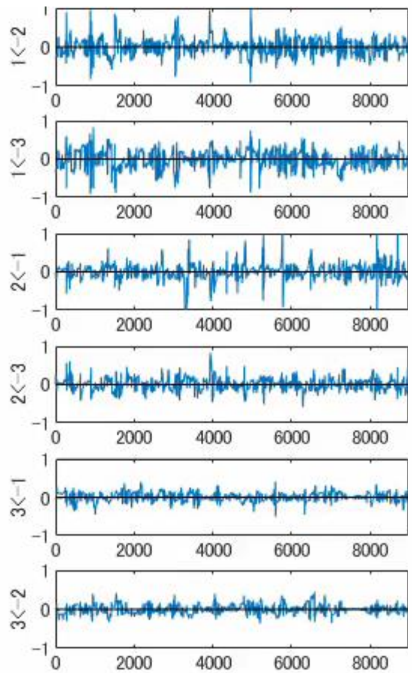
negative: repulsion

# Experiments (3) real-world mice data

(birds, bats, and flies are in our paper)

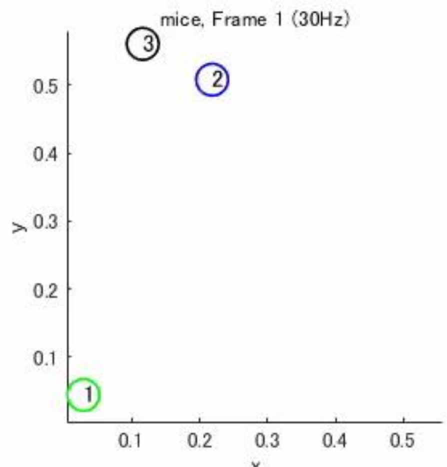
Raised in different cage

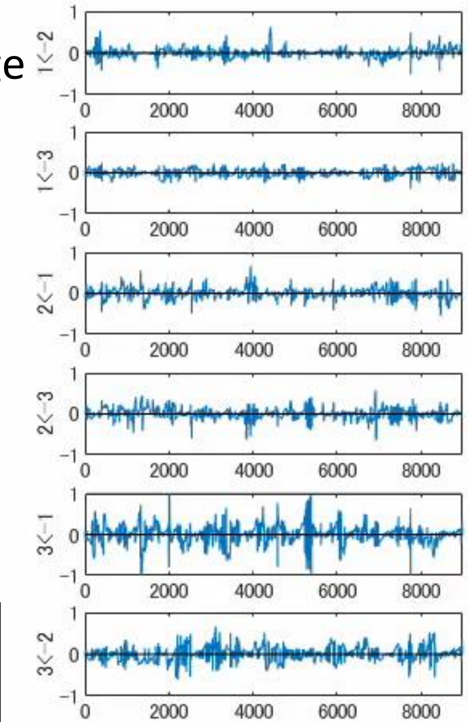



(30 Hz for 5 min)

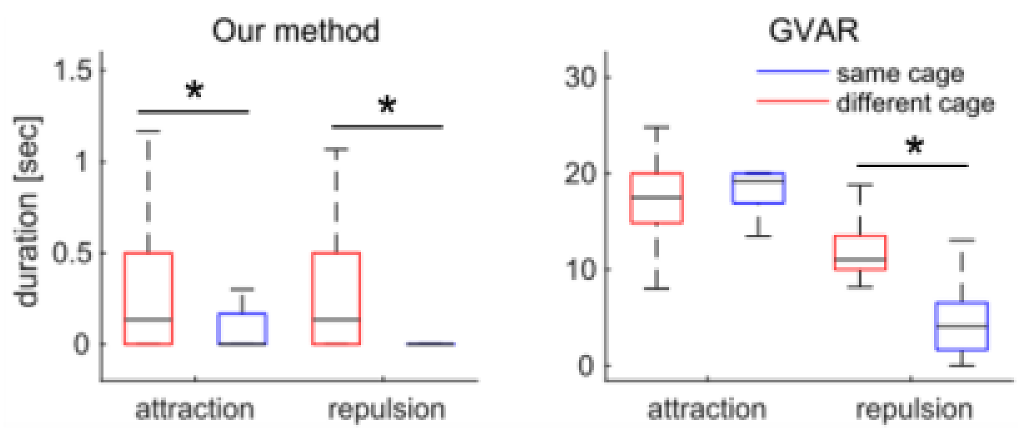
Raised in the same cage




positive: attraction
negative: repulsion

- Our method extracted a larger duration in the different cage than that in the same, whereas GVAR did too much interaction.
- Our methods characterized the movement behaviors before the contacts with others [Thanos+17]



# Conclusion

- We propose a framework for learning Granger causality via ABM, which can extract interaction rules from real-world multi-agent and multi-dimensional trajectory data
- We realized the theory-guided regularization for reliable biological behavioral modeling, which can leverage scientific knowledge such that "when this situation occurs, it would be like this"
- Biologically, we reformulate a well-known conceptual behavioral model, which did not have a numerically computable form, such that we can compute and quantitatively evaluate it
- Our method achieved better performance than various baselines using synthetic datasets, and obtained new biological insights using multiple datasets of mice, birds, bats, and flies

Acknowledgments: This work was supported by JSPS KAKENHI (Grant Numbers 19H04941, 20H04075, 16H06541, 25281056, 21H05296, 18H03786, 21H05295, 19H04939, JP18H03287, and 21H05300), JST PRESTO (JPMJPR20CA), and JST CREST (JPMJCR1913). For obtaining flies data, we would like to thank Ryota Nishimura at Nagoya Univ.