appliedAI institute for europe

Mind the Gap: Methods and Applicability of Simulation-Based Inference

Transfer Lab Seminar | March 14th, 2024 | Munich

A joint initiative | UNTERNEHMERTUM | IPAI

Computer simulations in science

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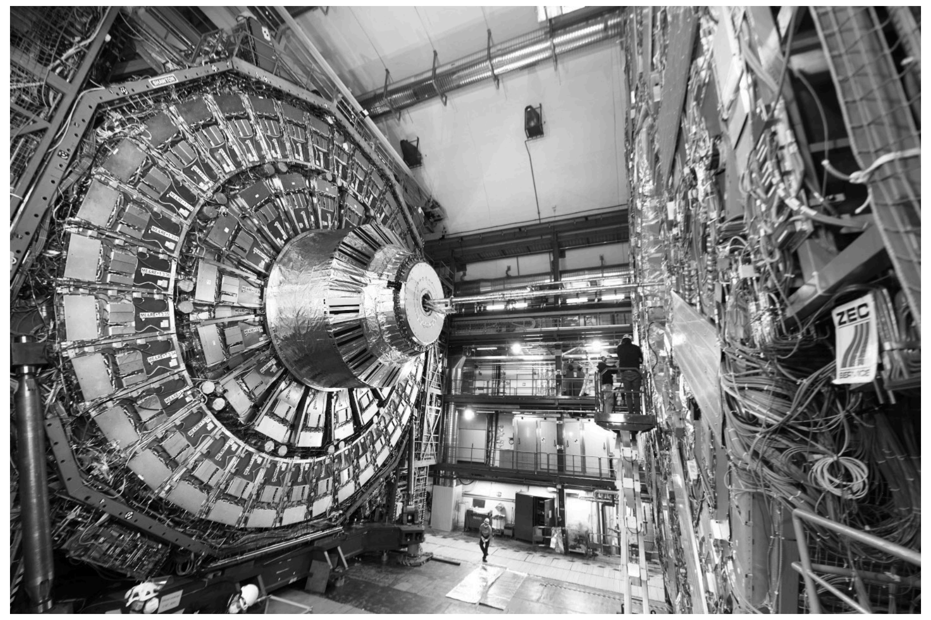
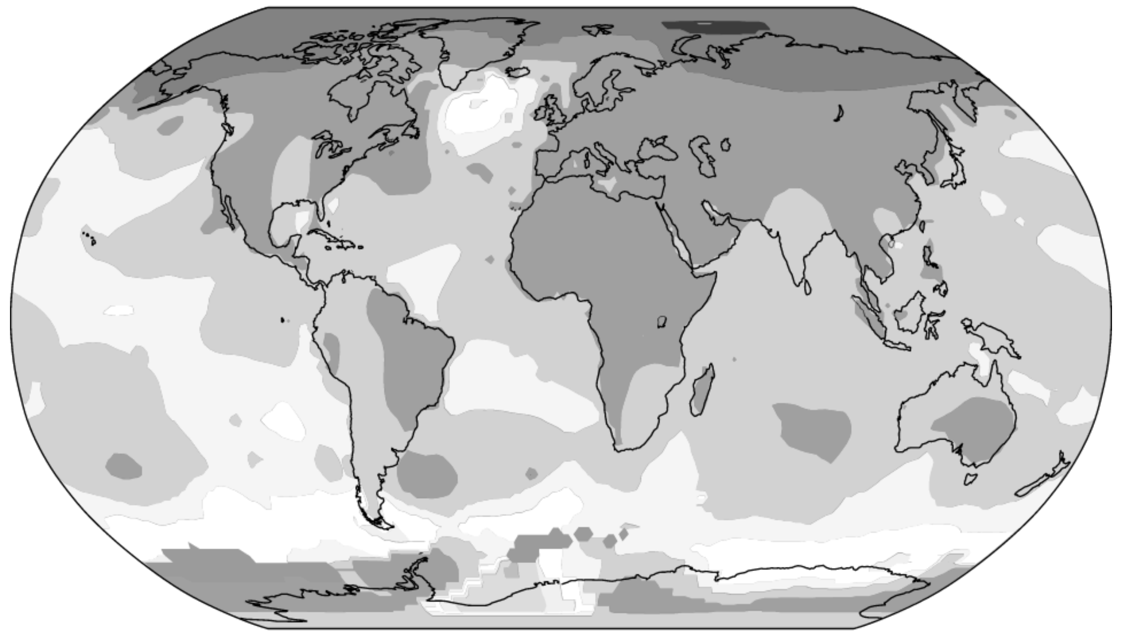


particle physics

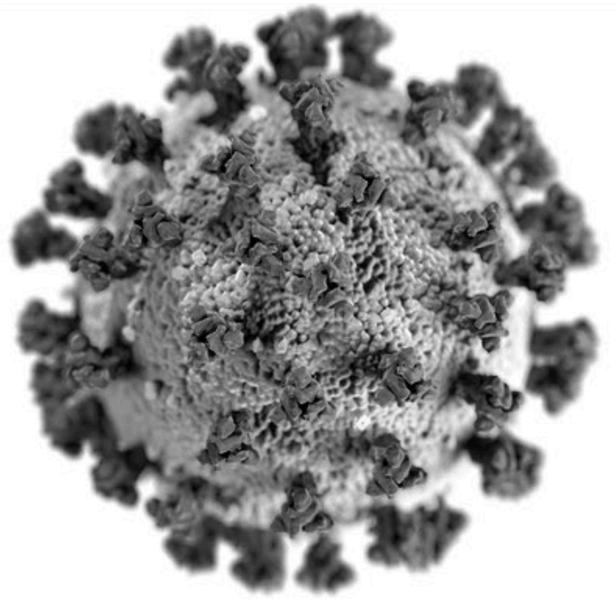
neuroscience



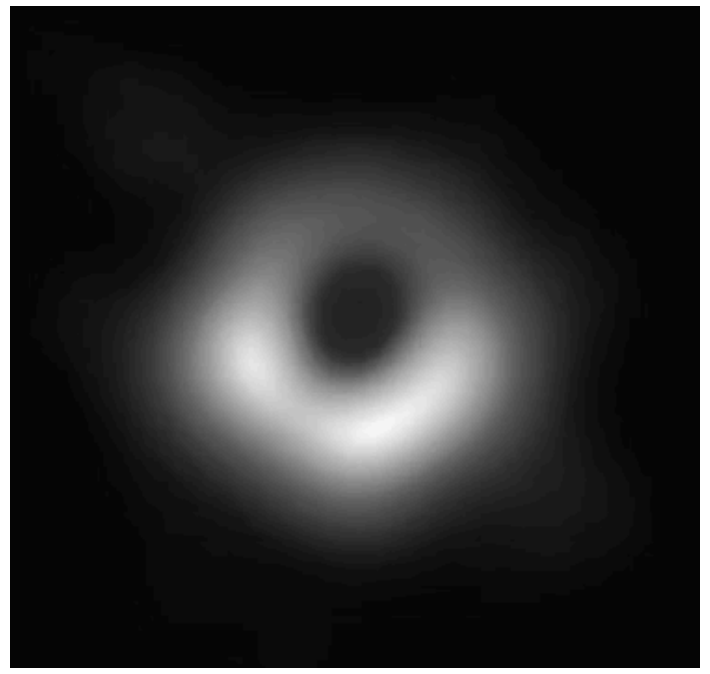
climate science

genomics

epidemiology



astrophysics



CERN; getty images; Wikipedia

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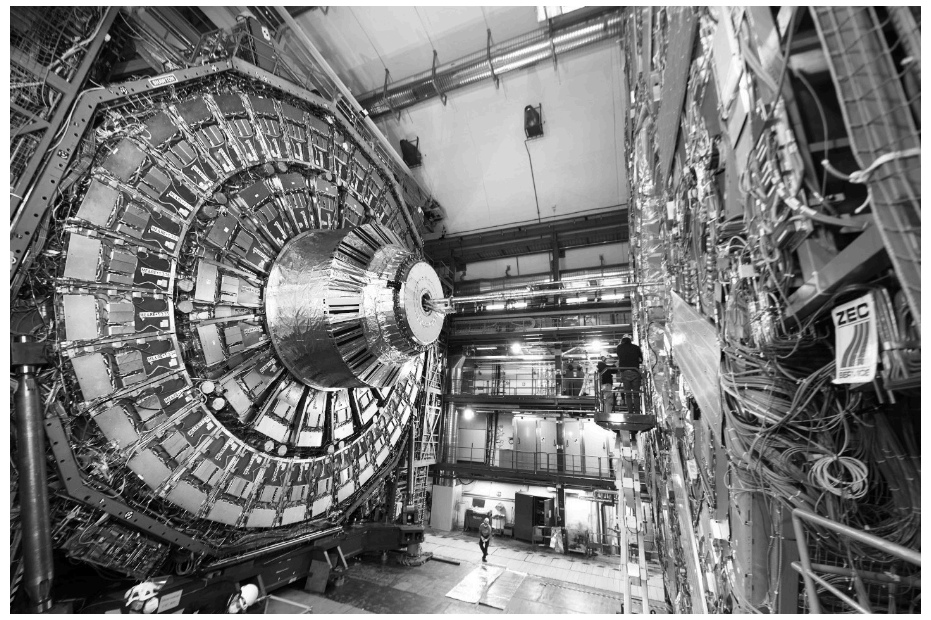

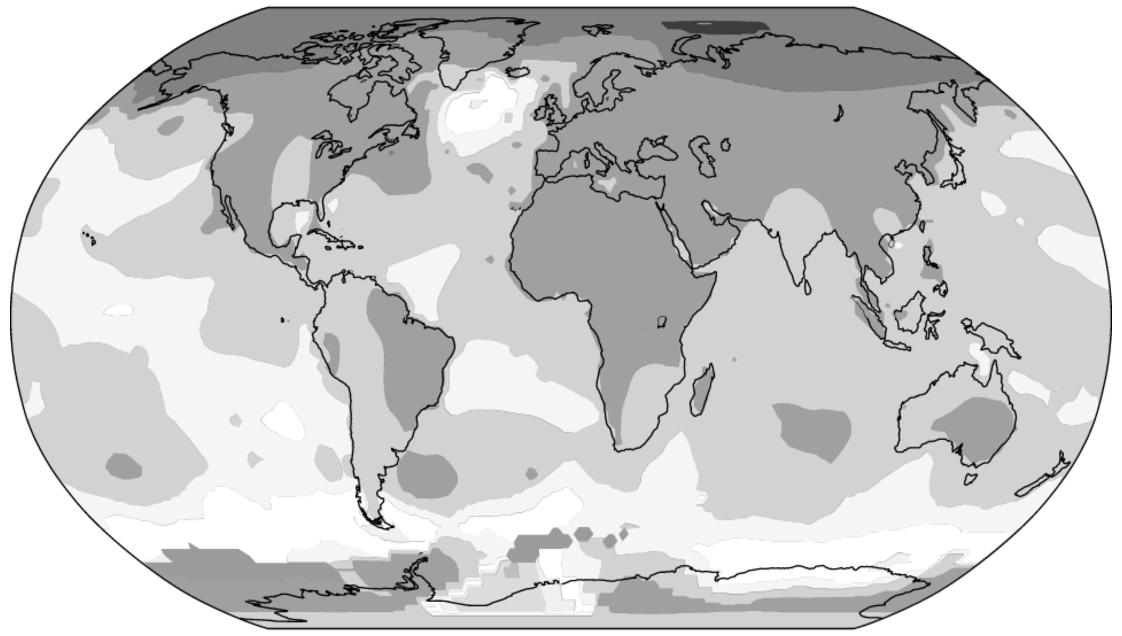

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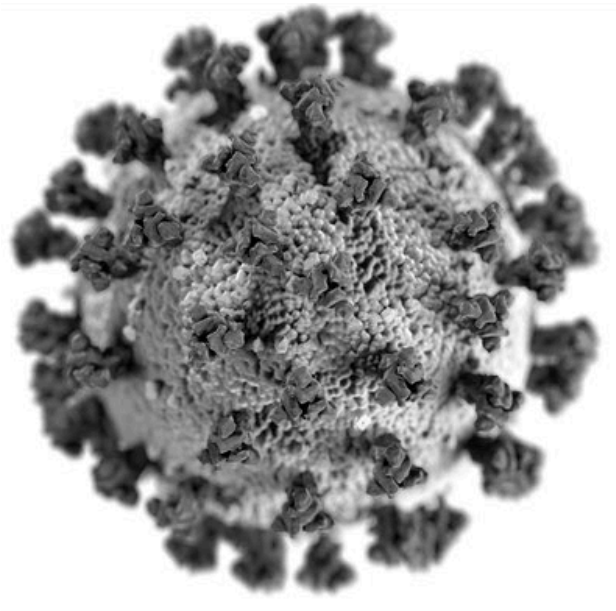

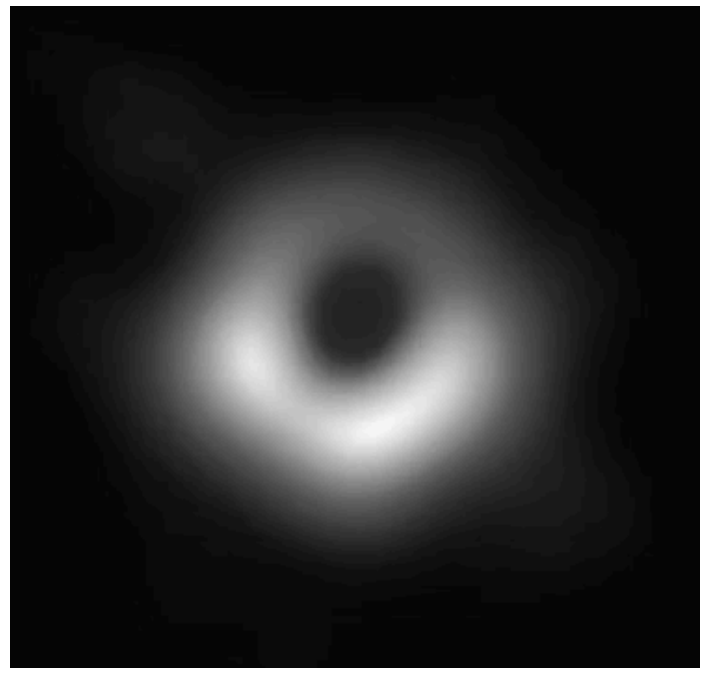

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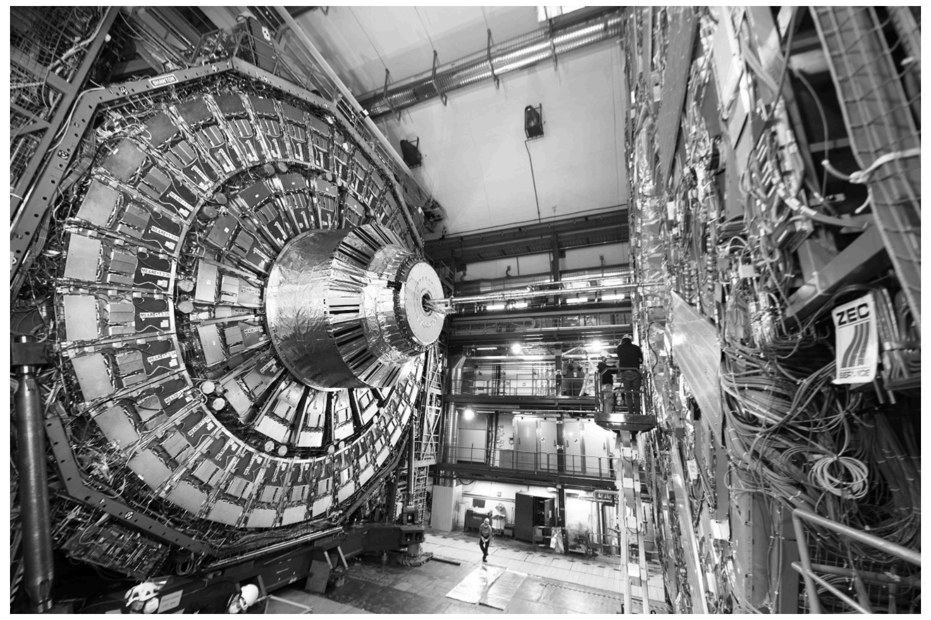

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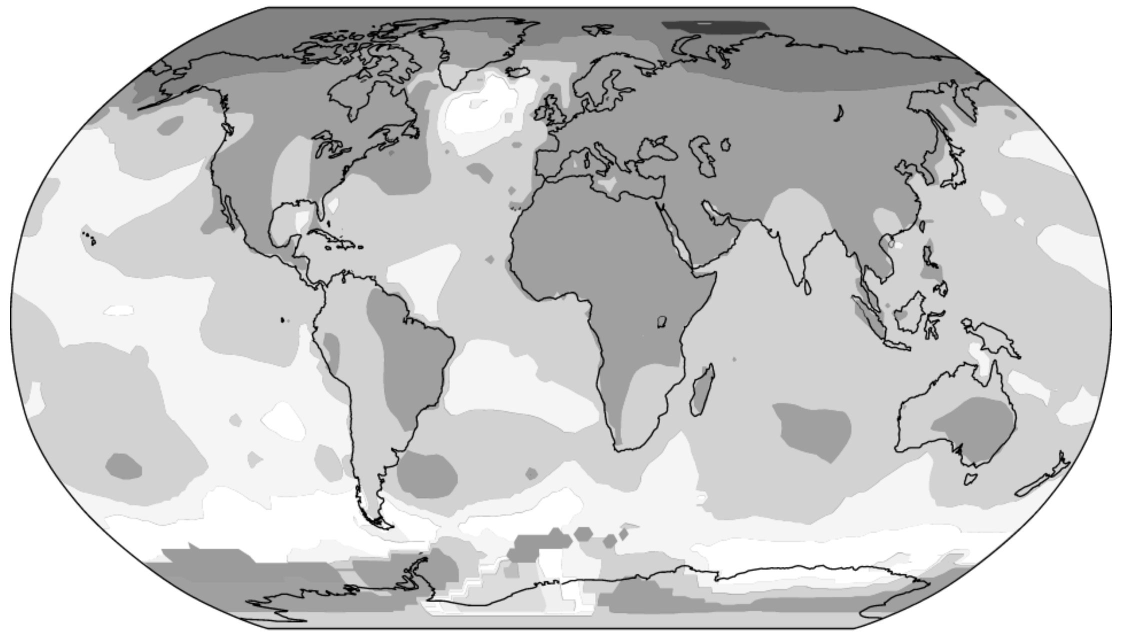

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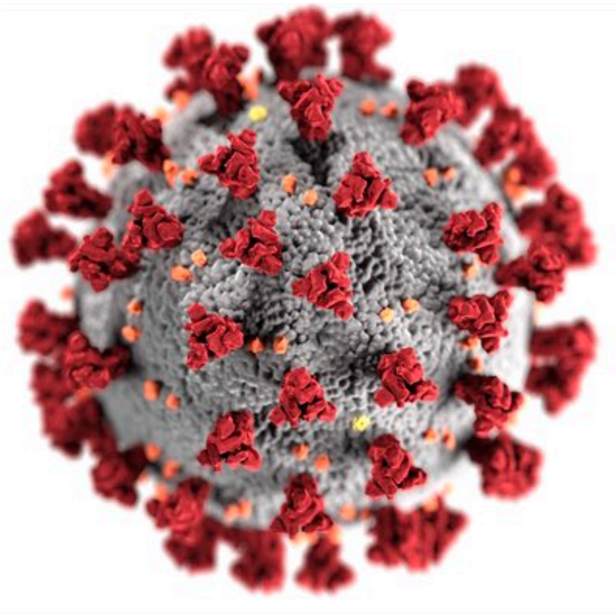

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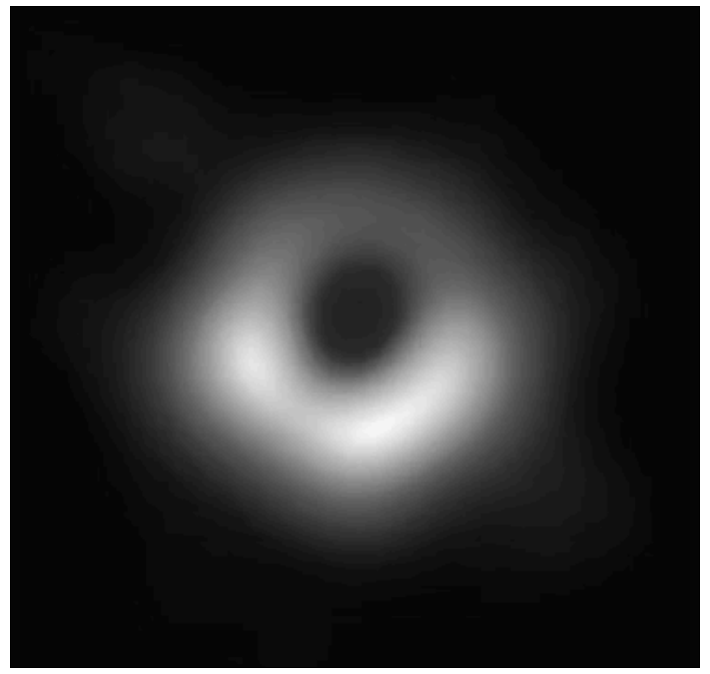

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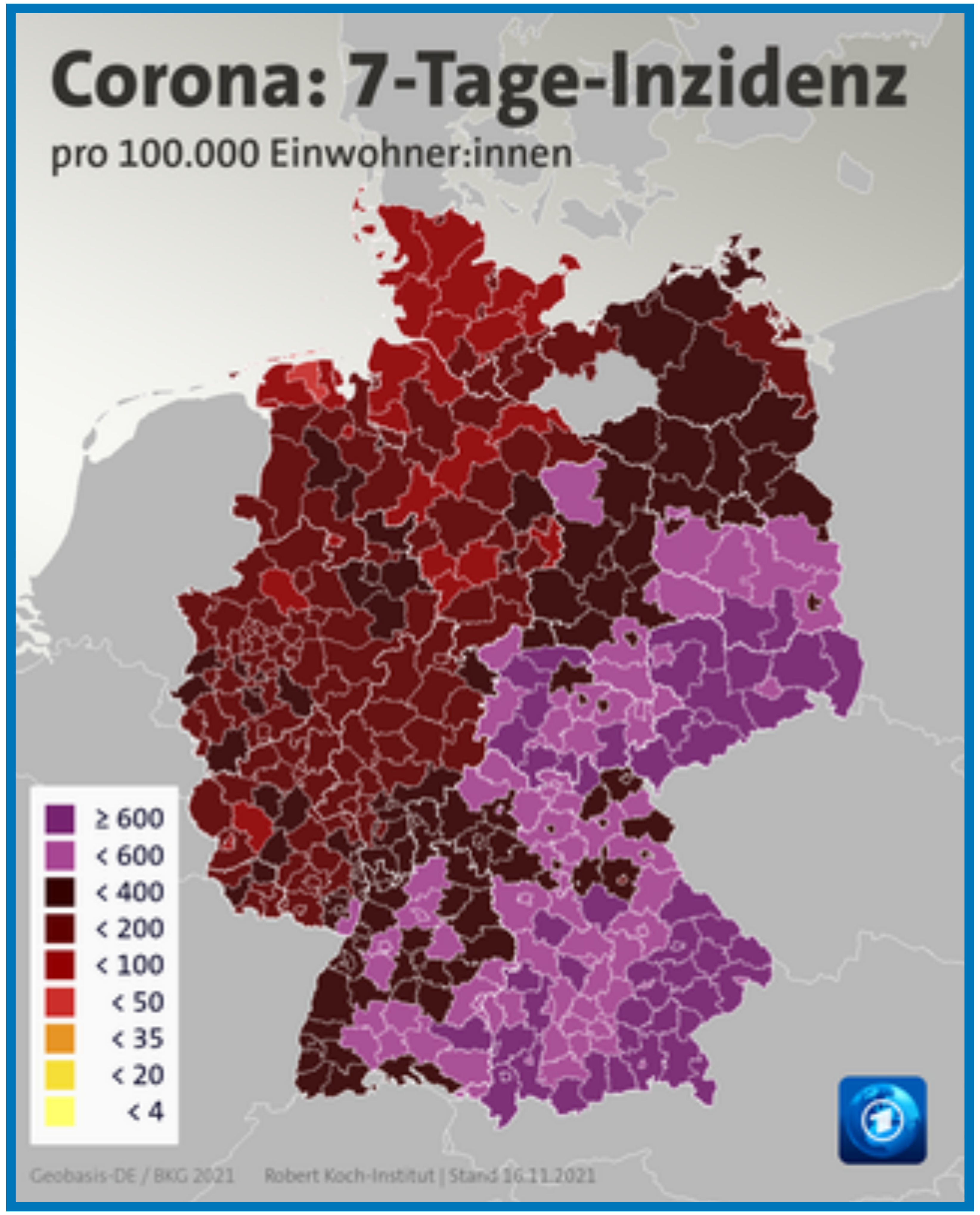
Simulations during the covid-19 pandemic



tagesschau.de, 2021; Dehning et al. 2020, Science

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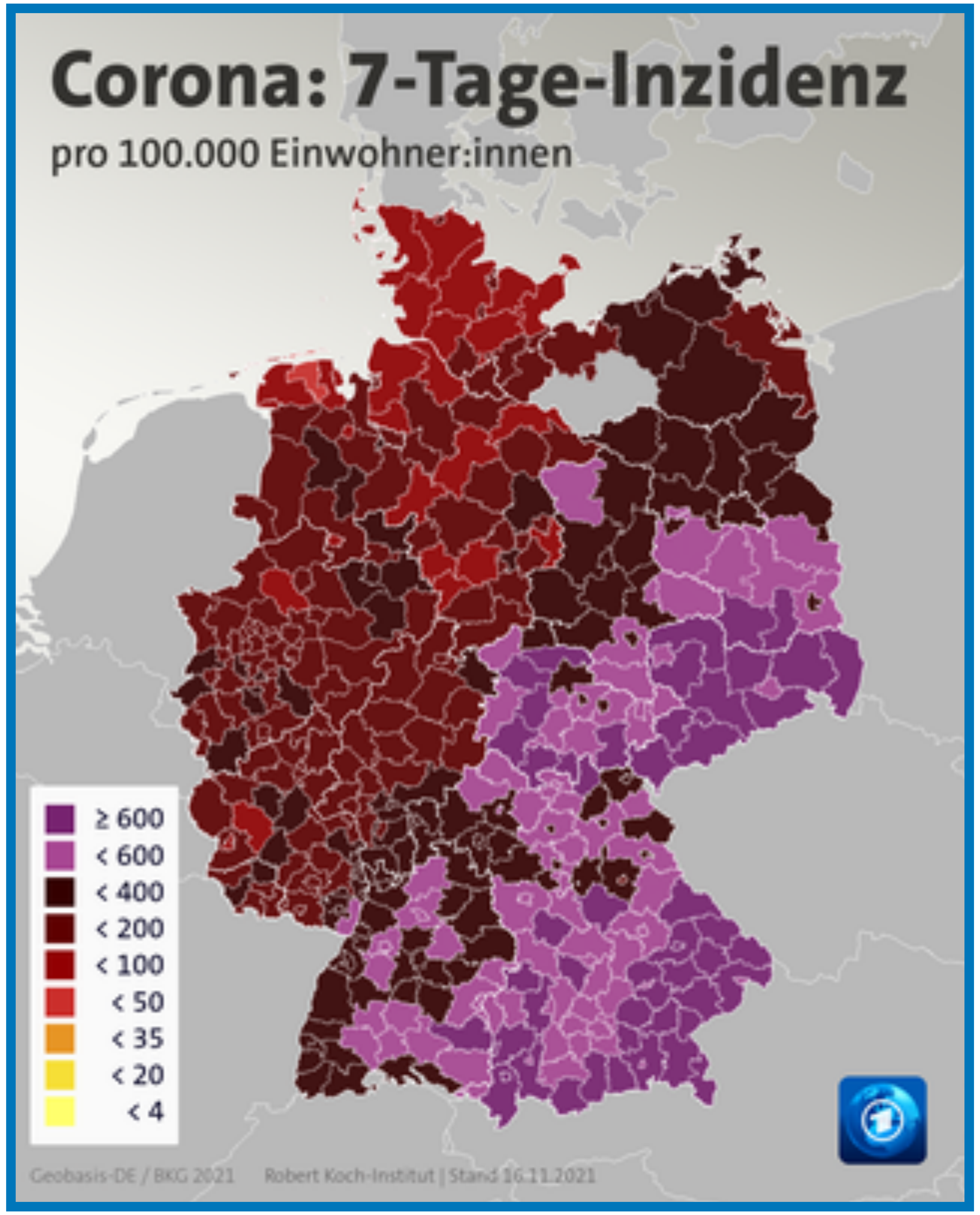

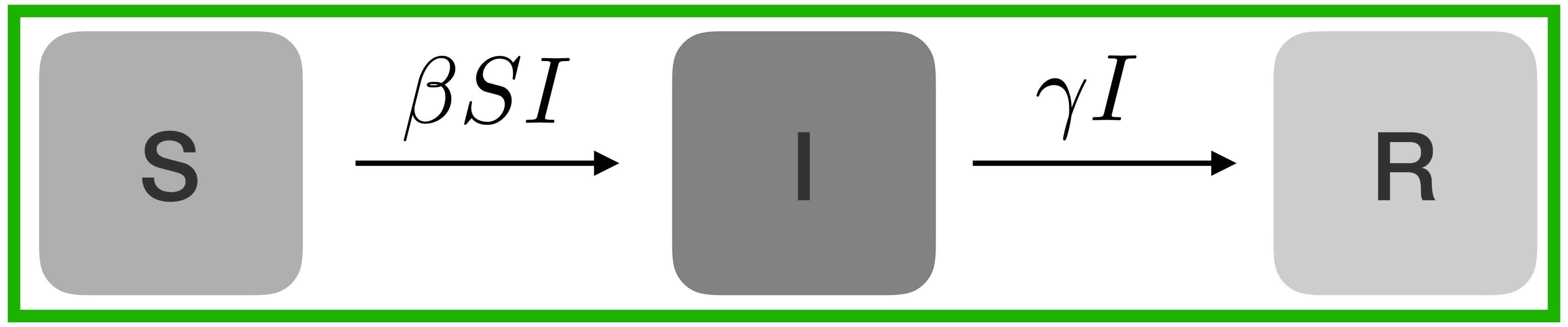

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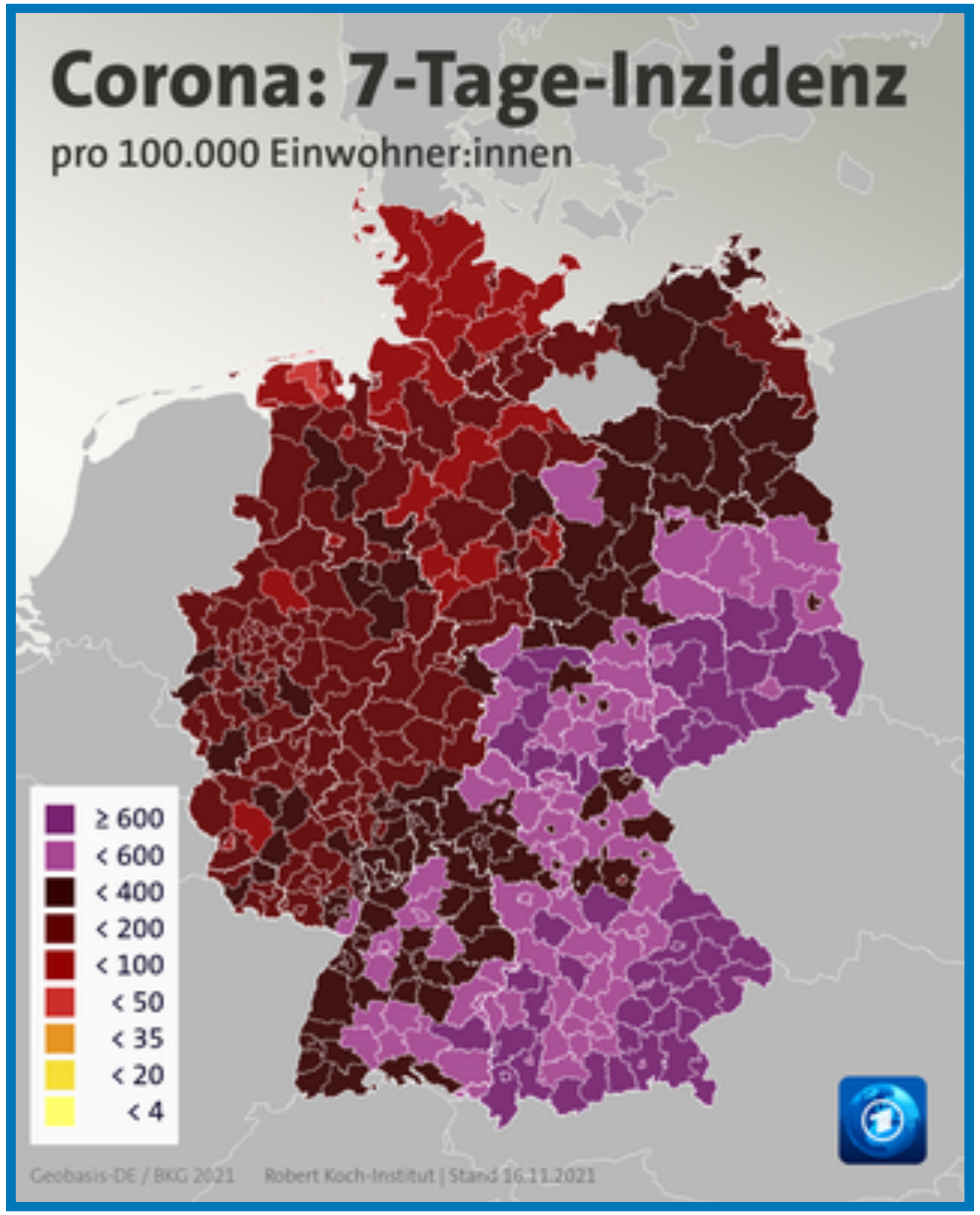

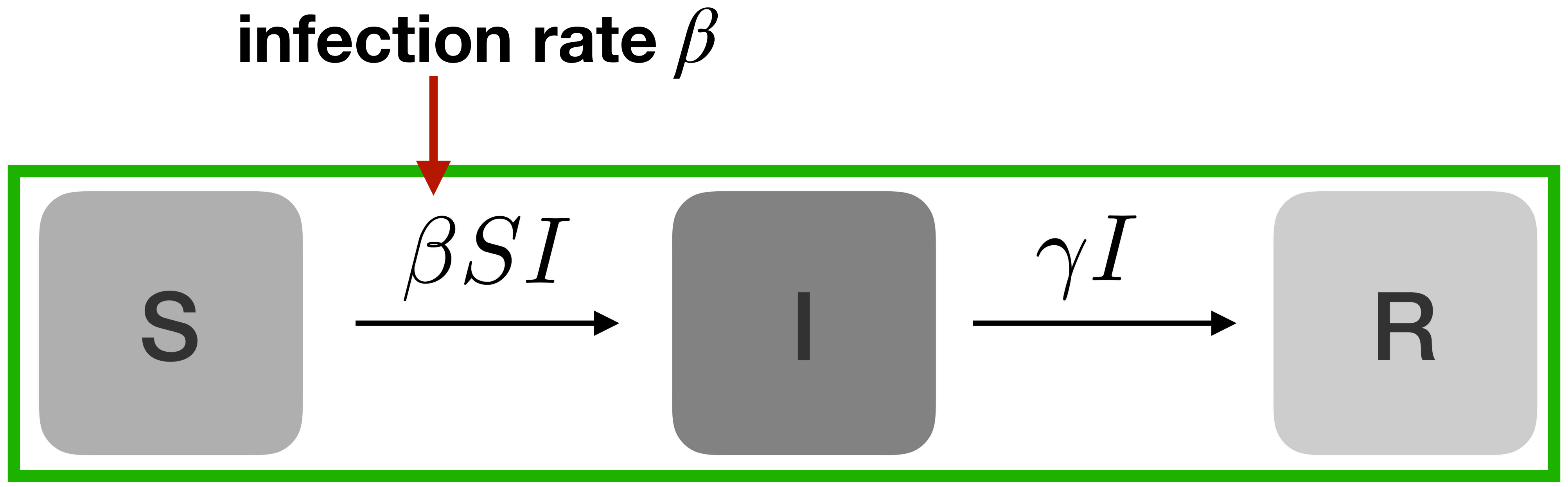

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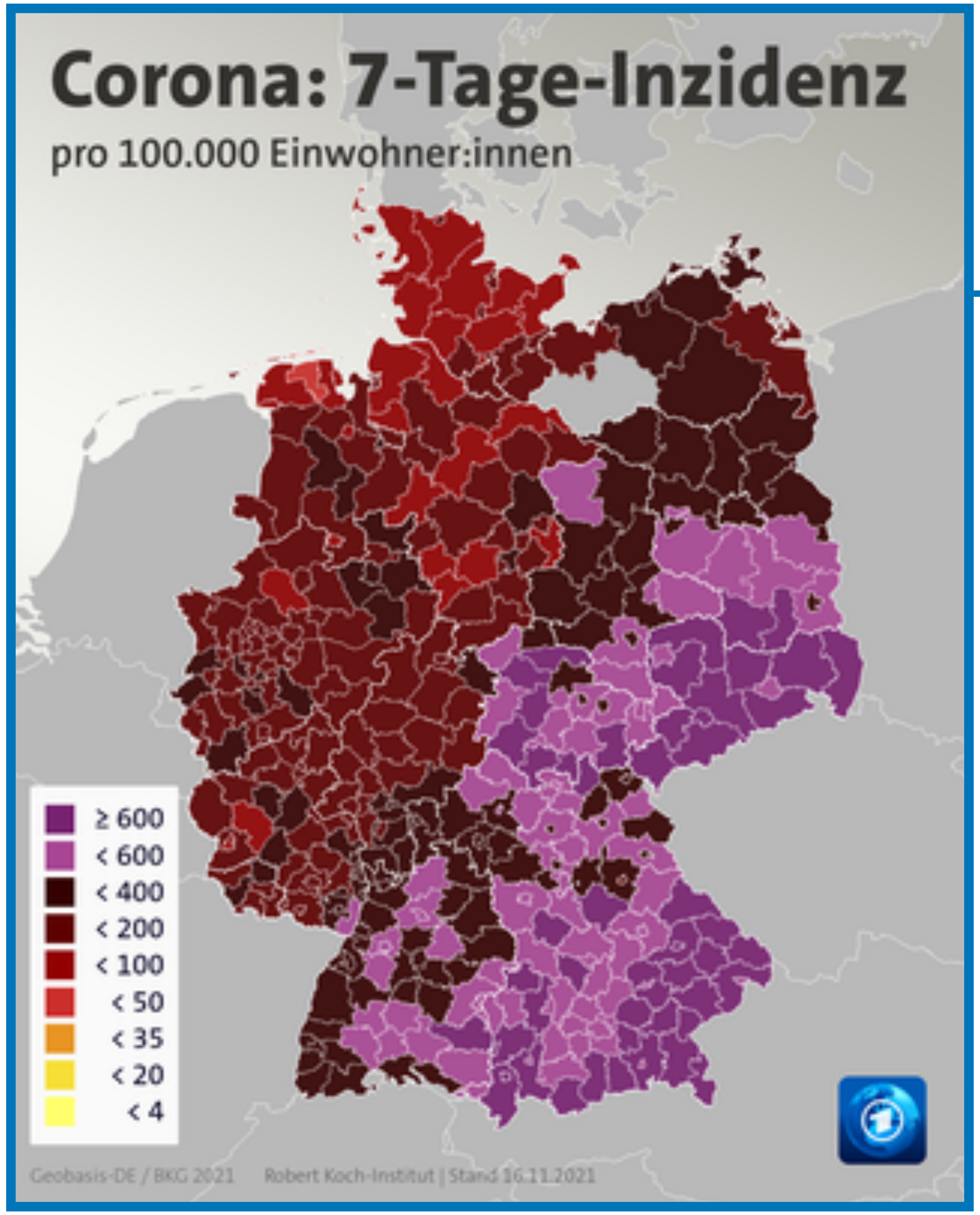

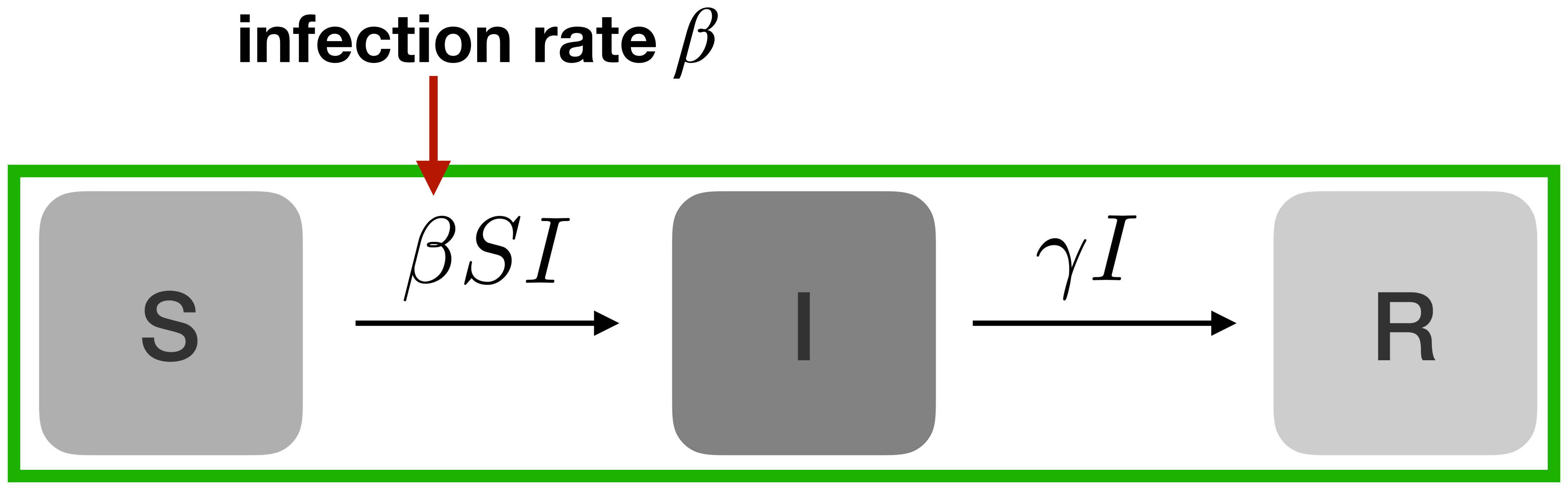

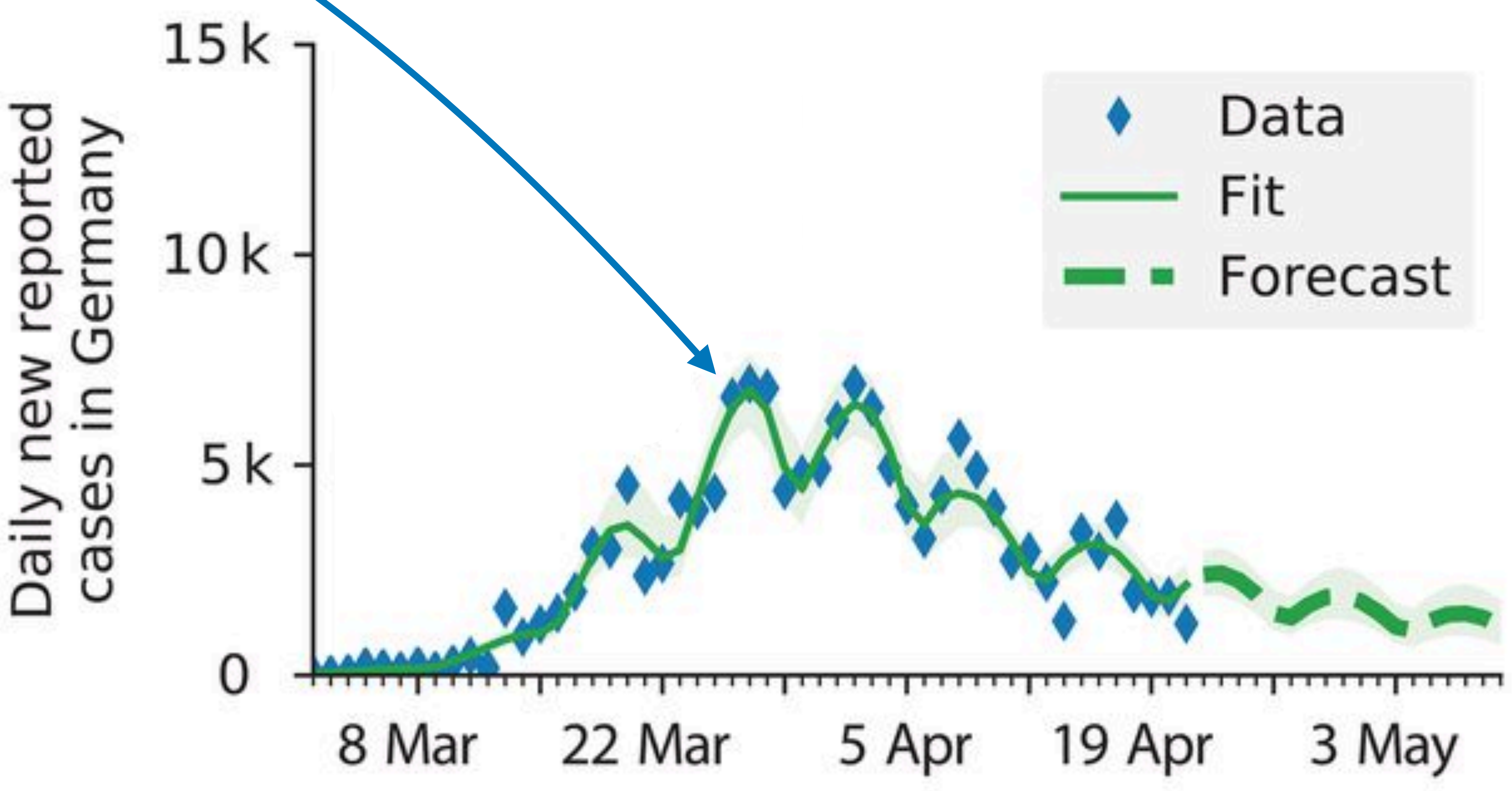

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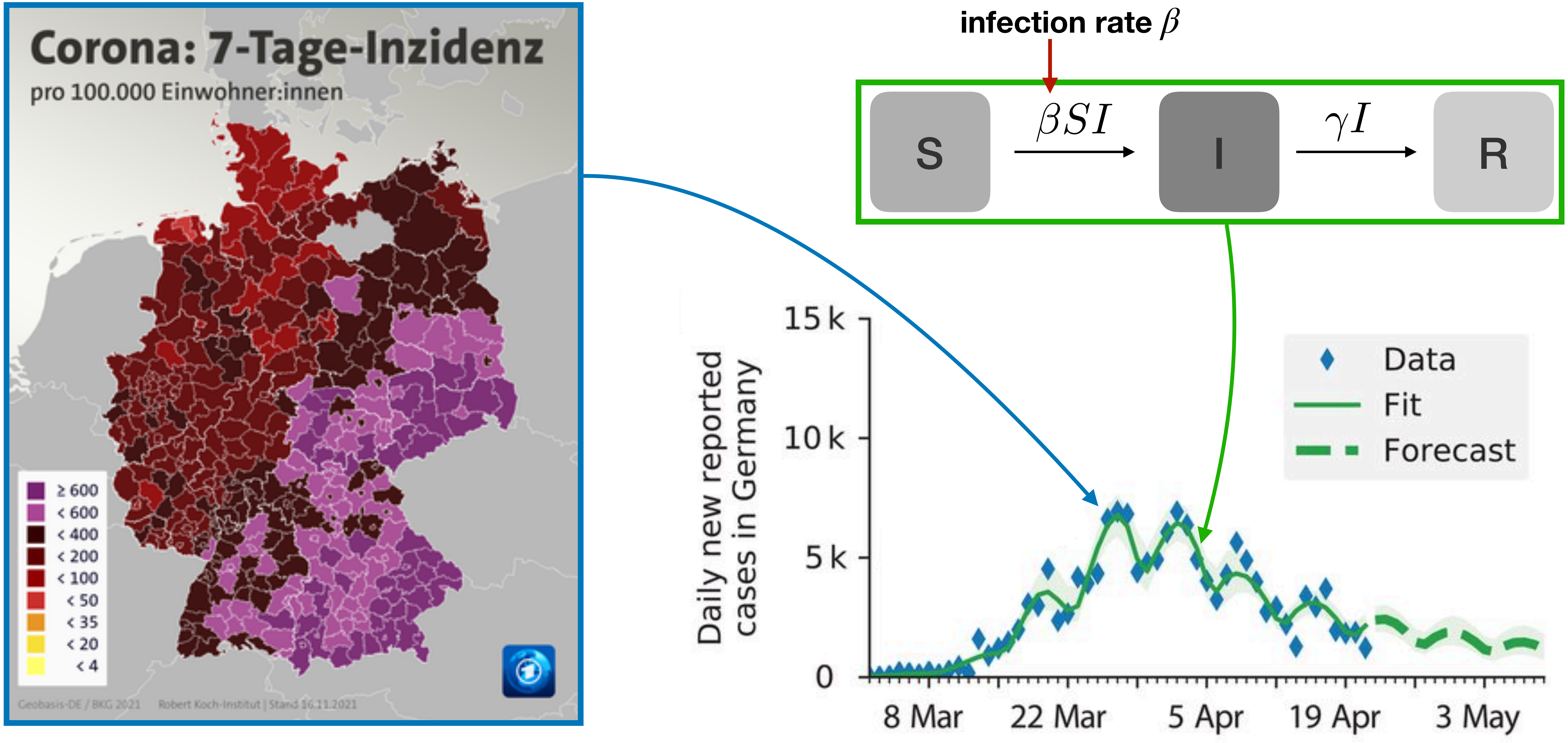

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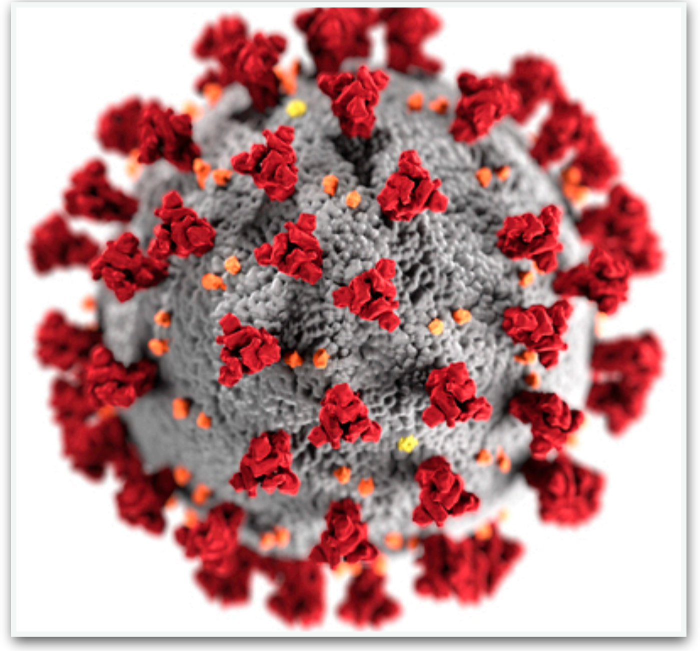
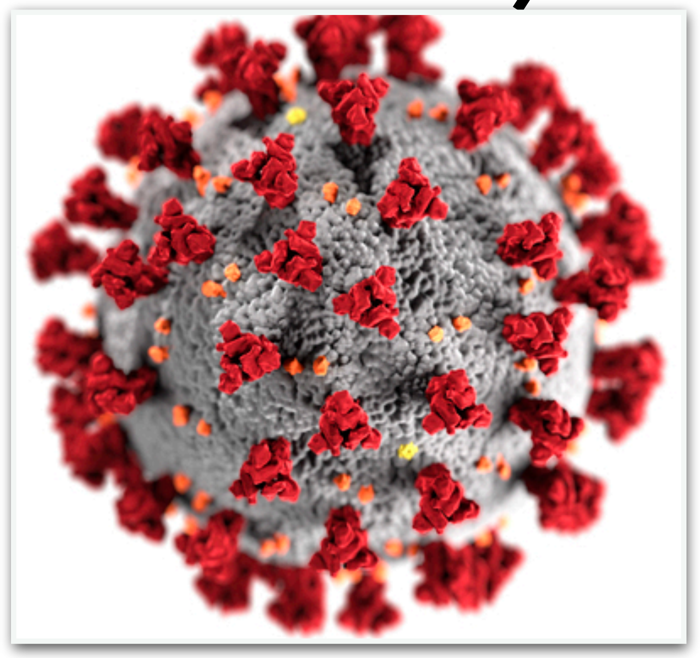
The simulation-based modeling approach

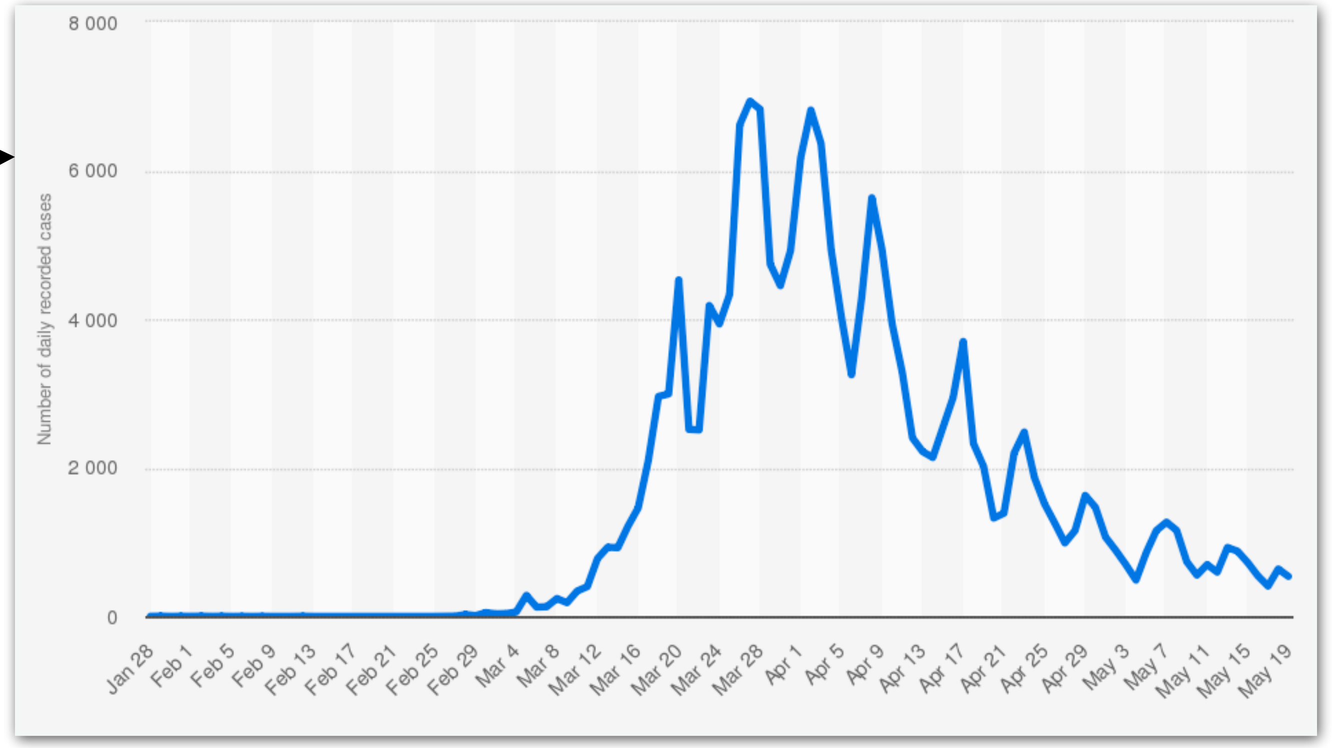


Paul Ehrlich Institut; WHO; Dehning et al. 2020

The simulation-based modeling approach

observe data





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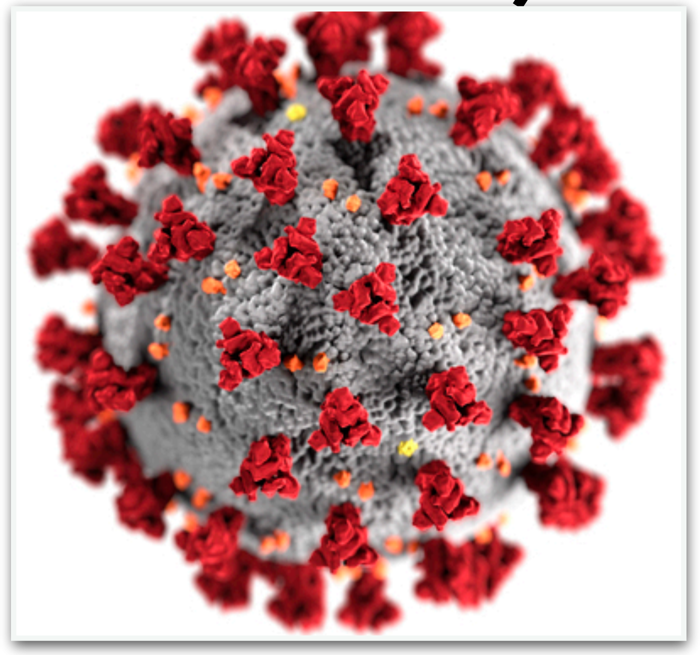
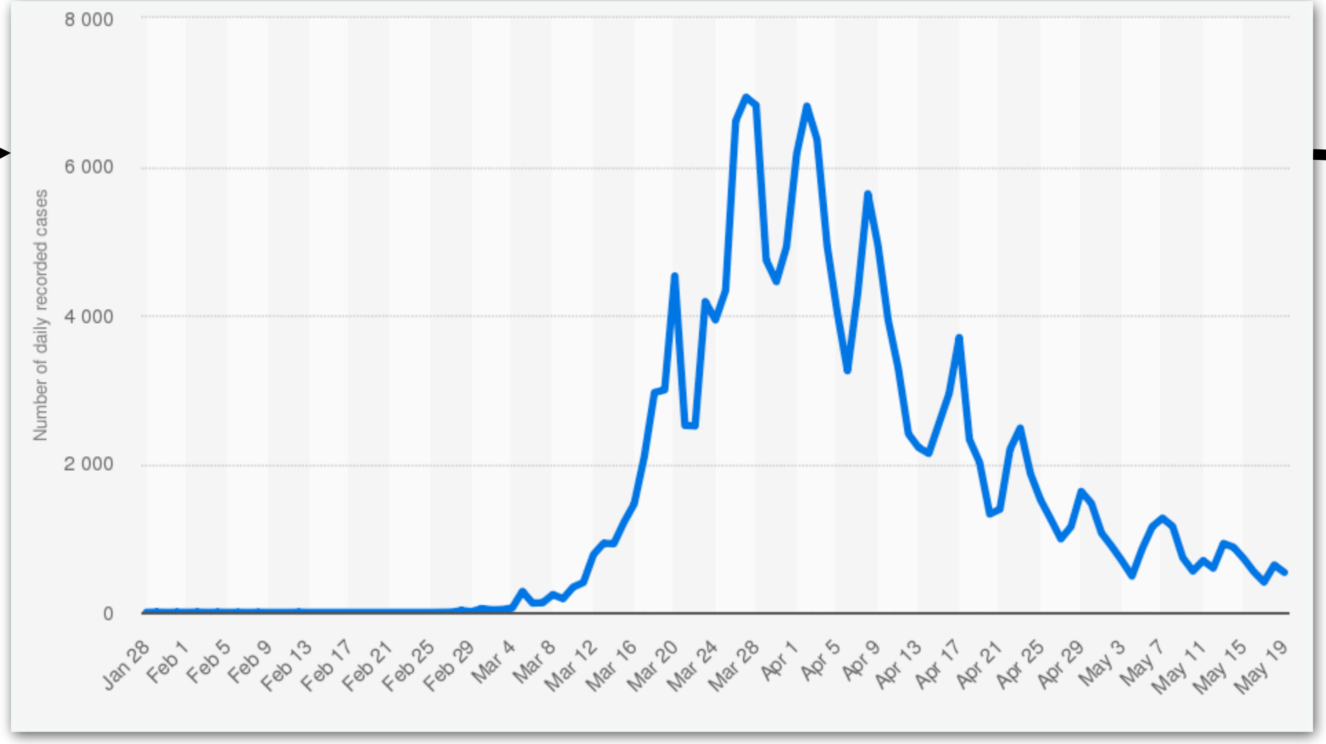
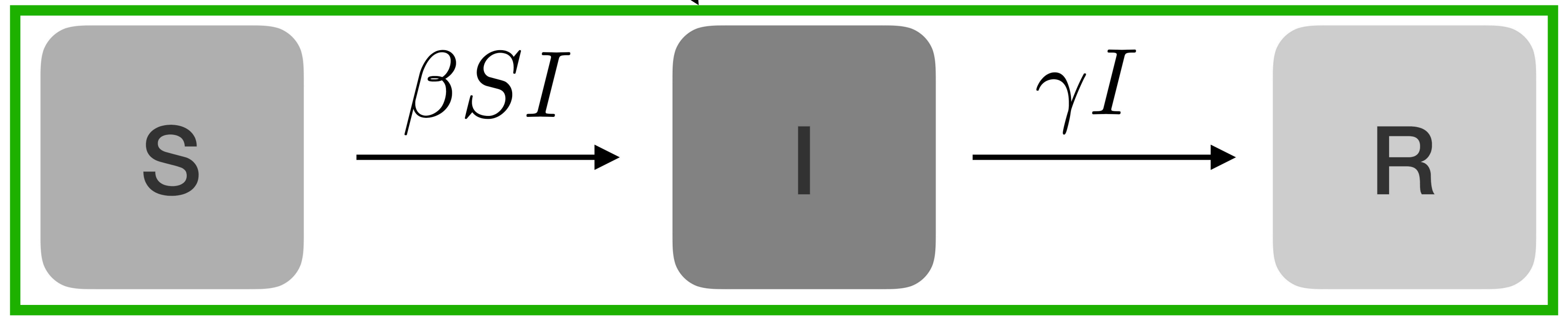




build a model



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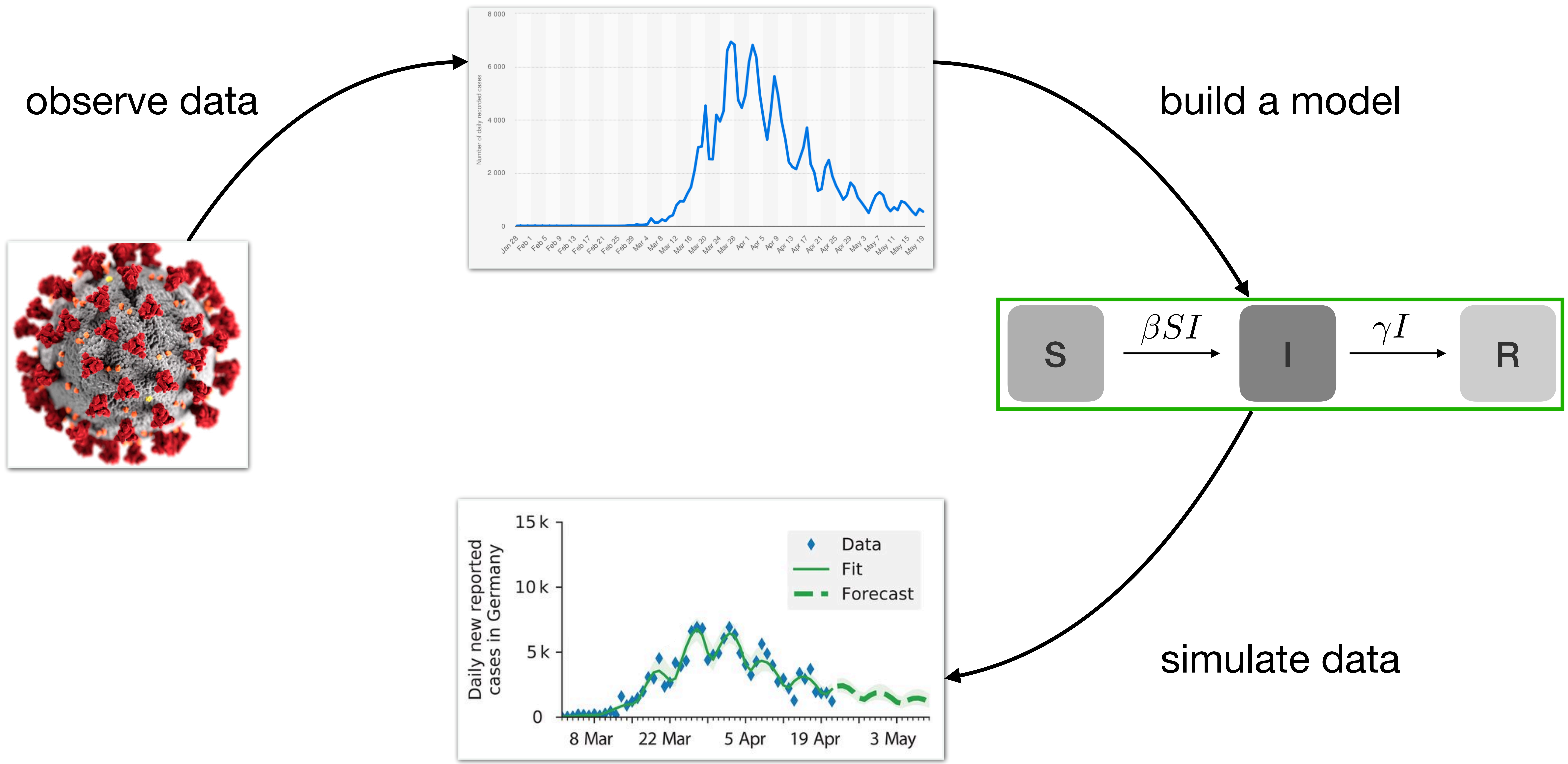

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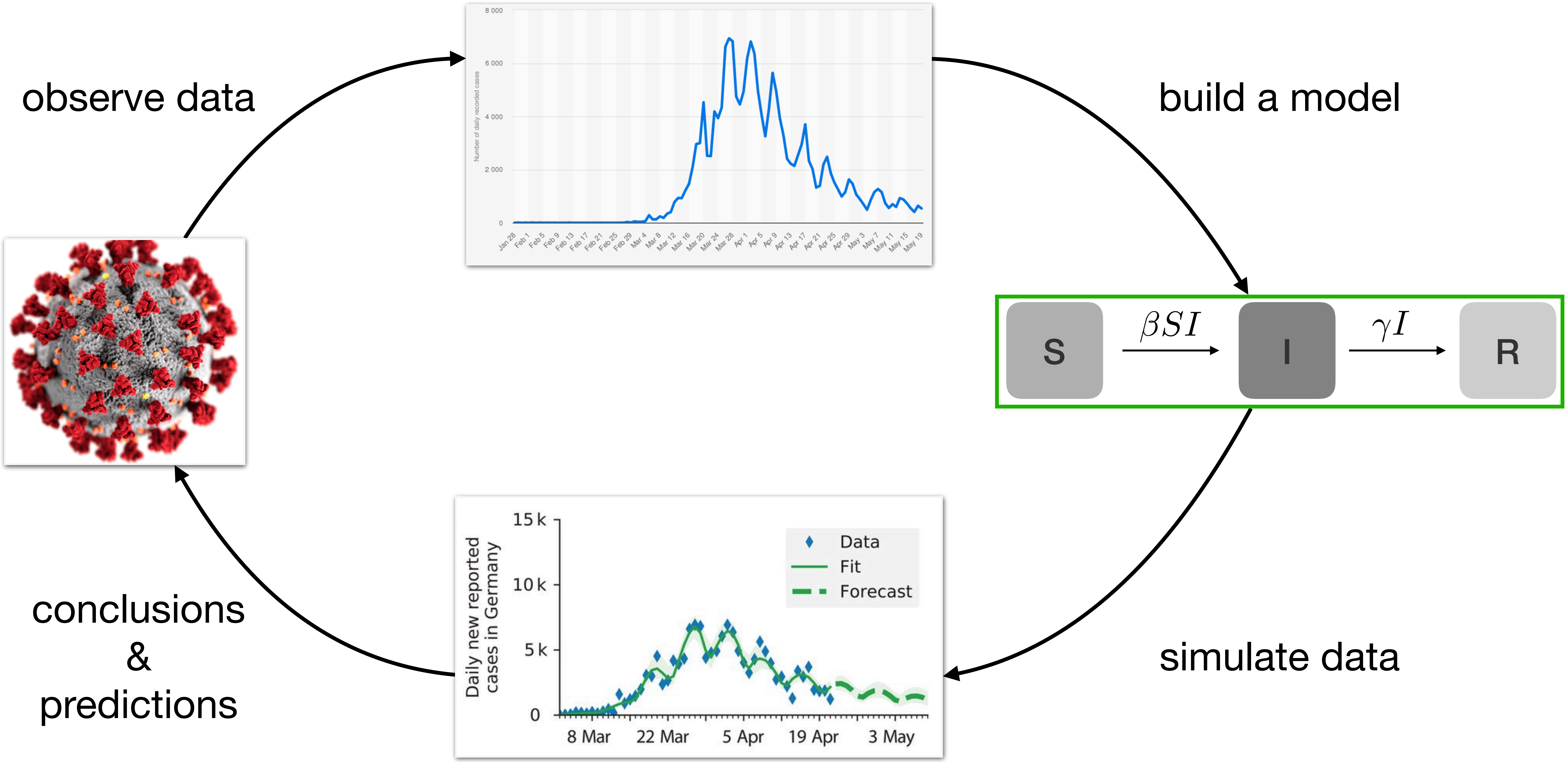

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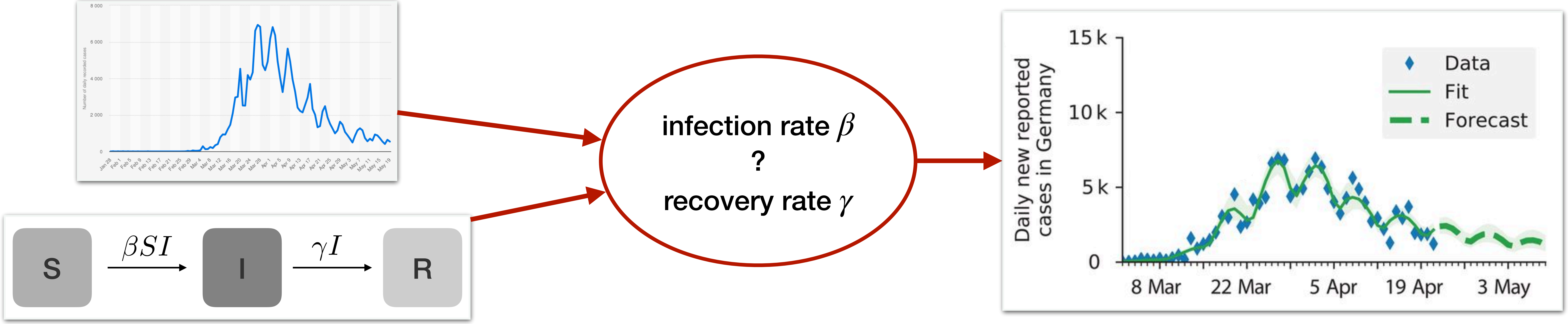
Central challenge: finding model parameters



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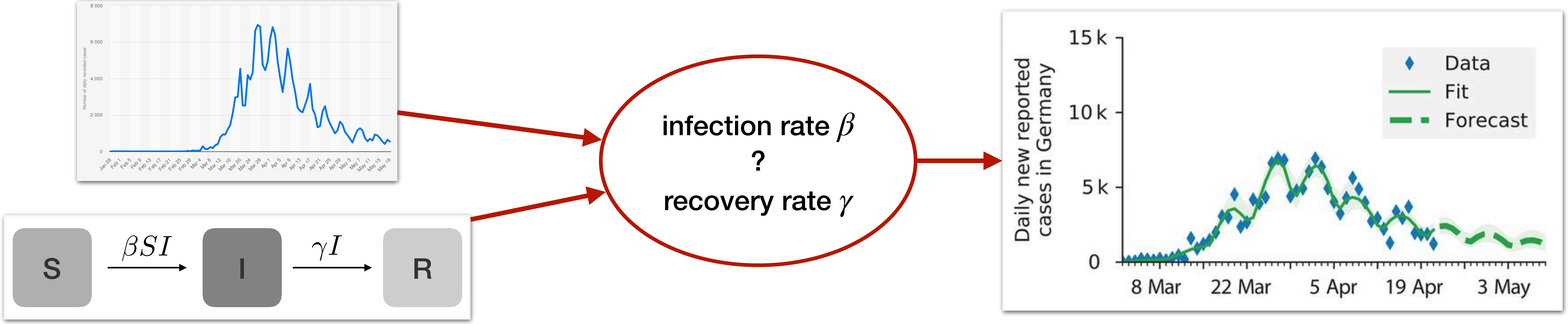
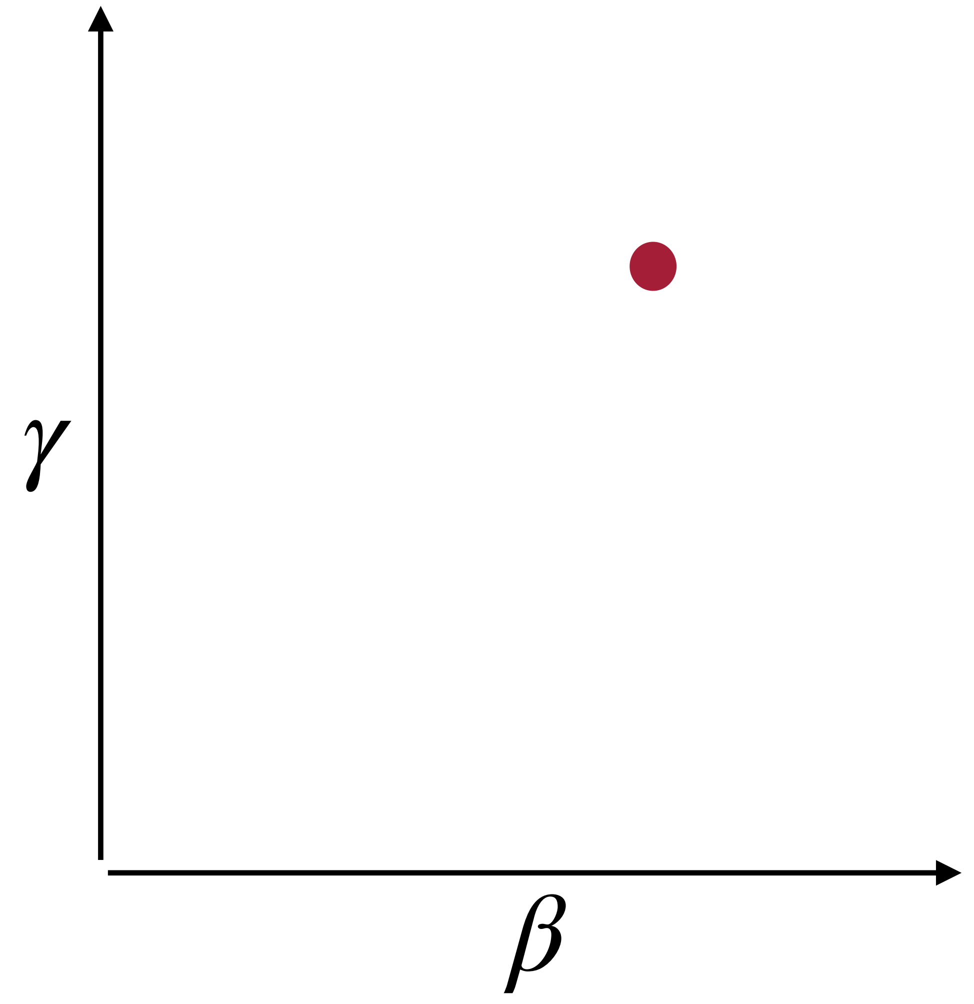


Naive approach

- find single best-fitting parameters
  - hand tuning
  - grid search



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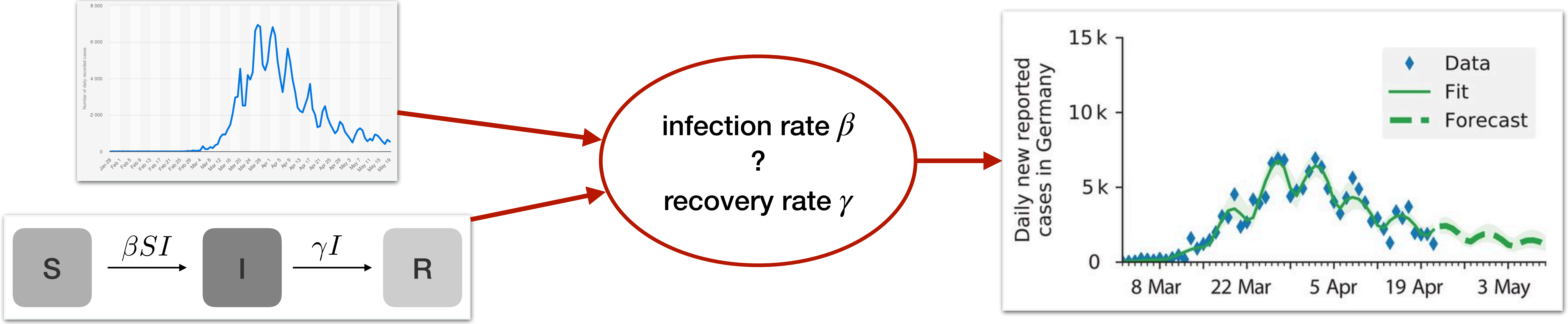

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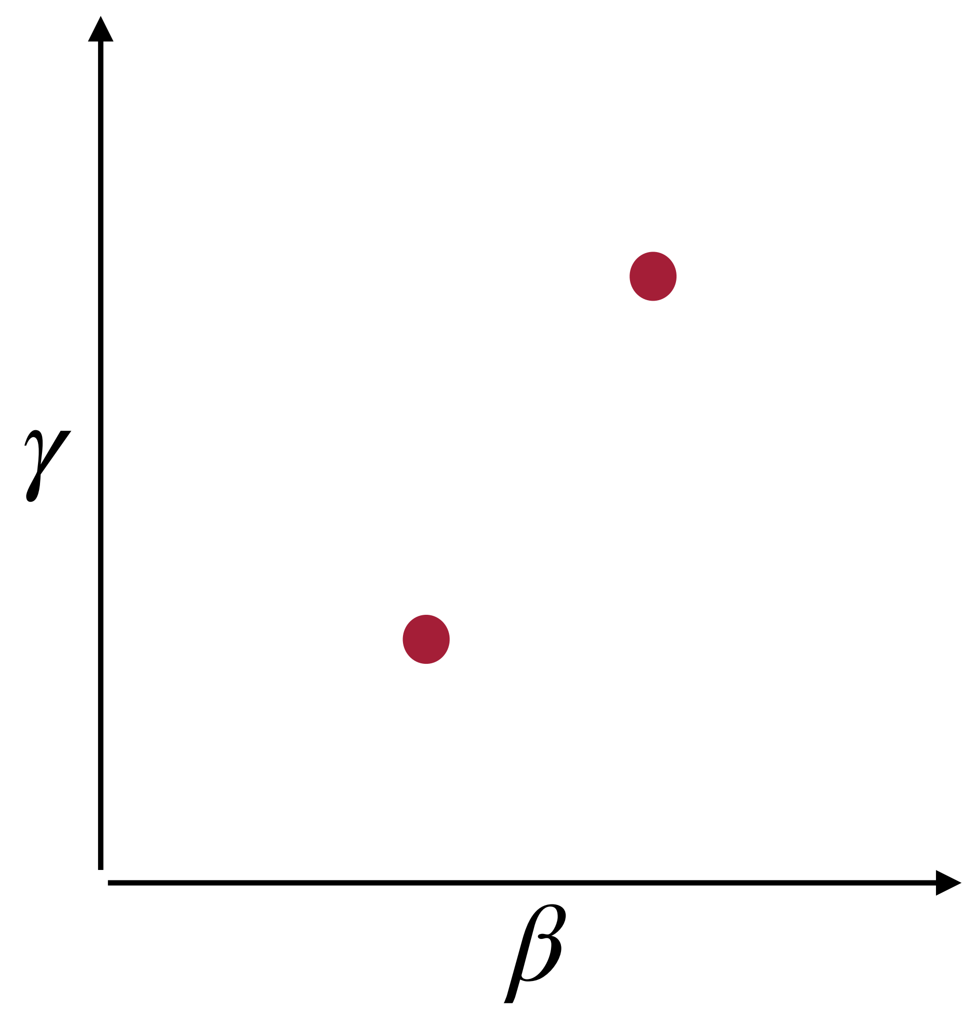

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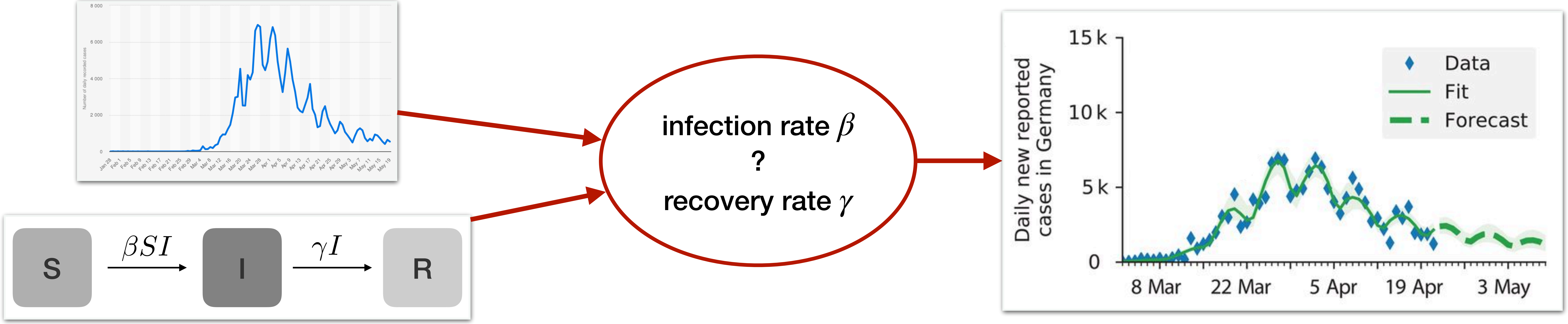

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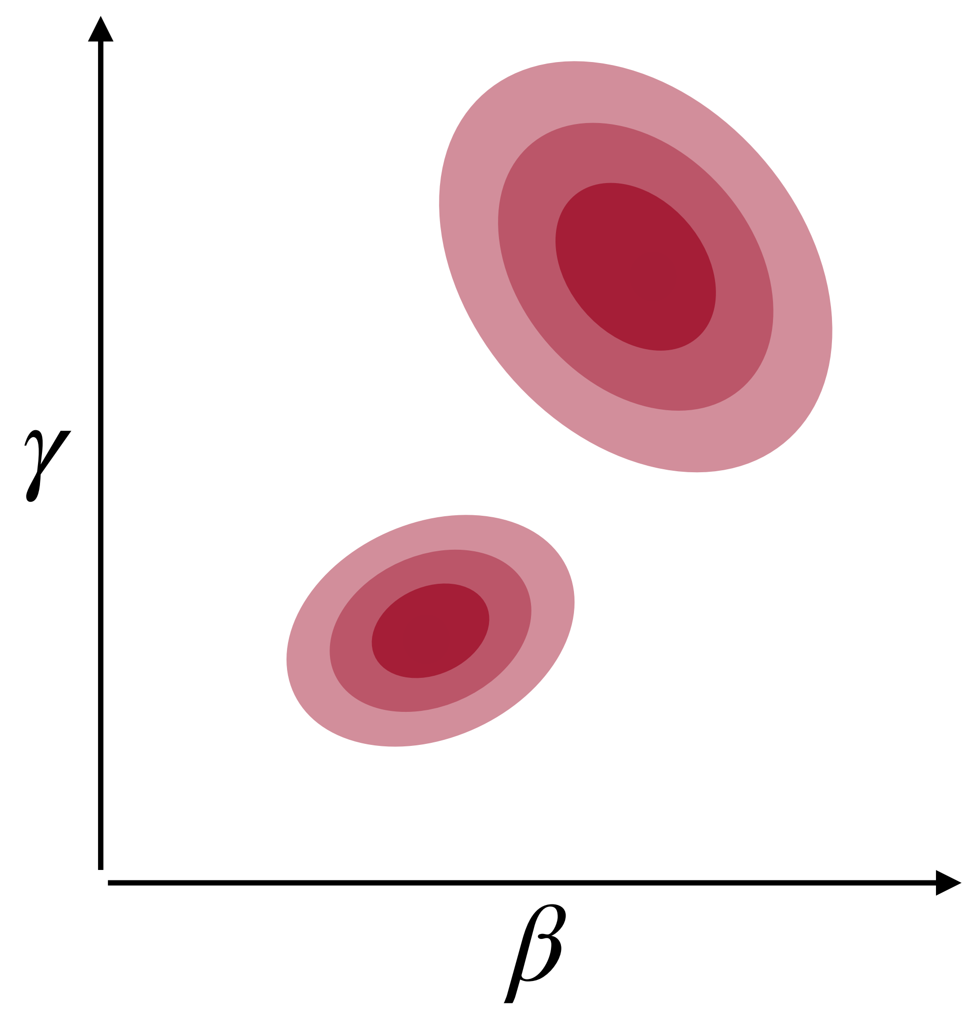

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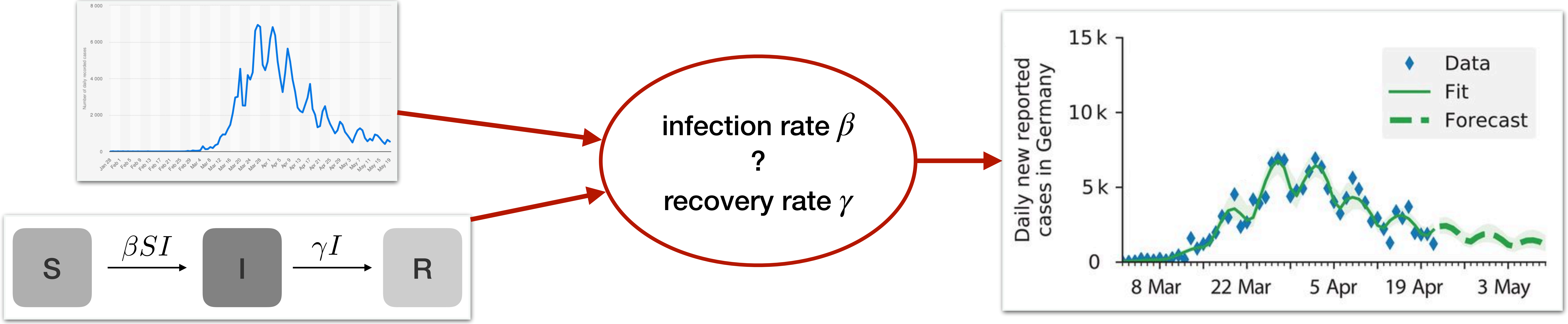

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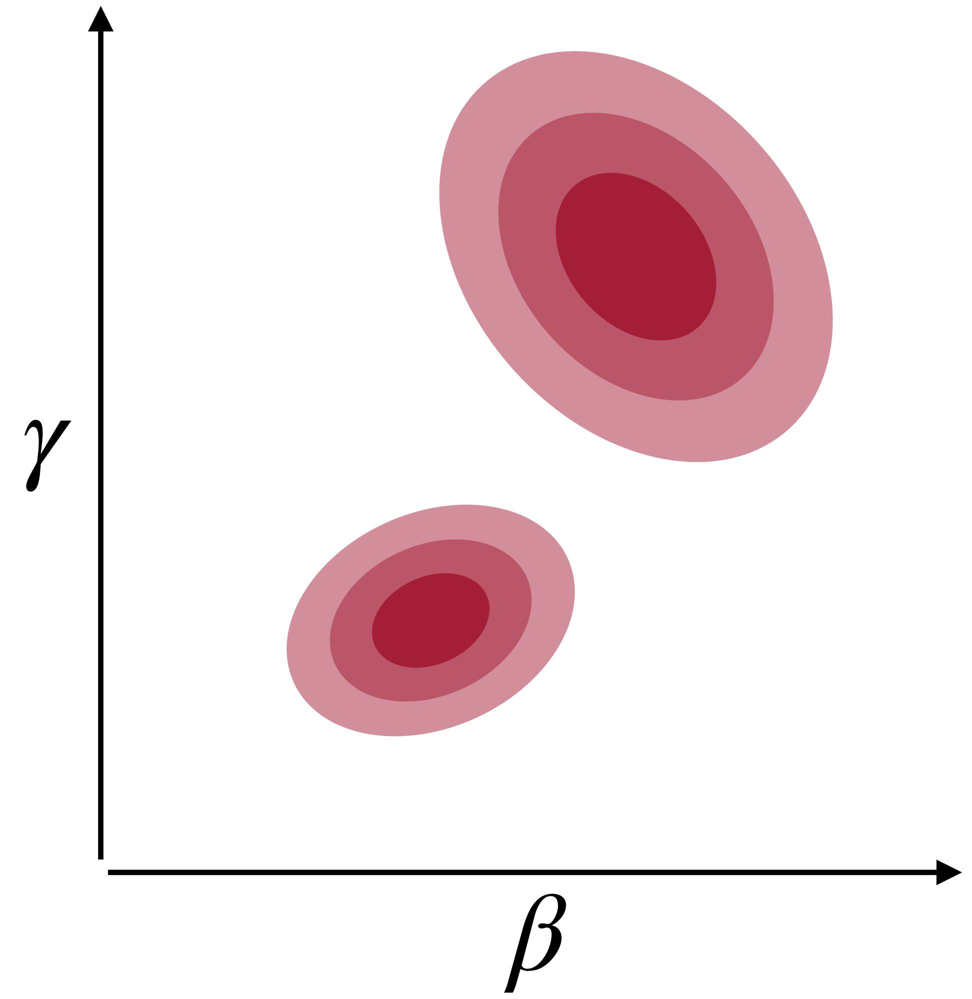
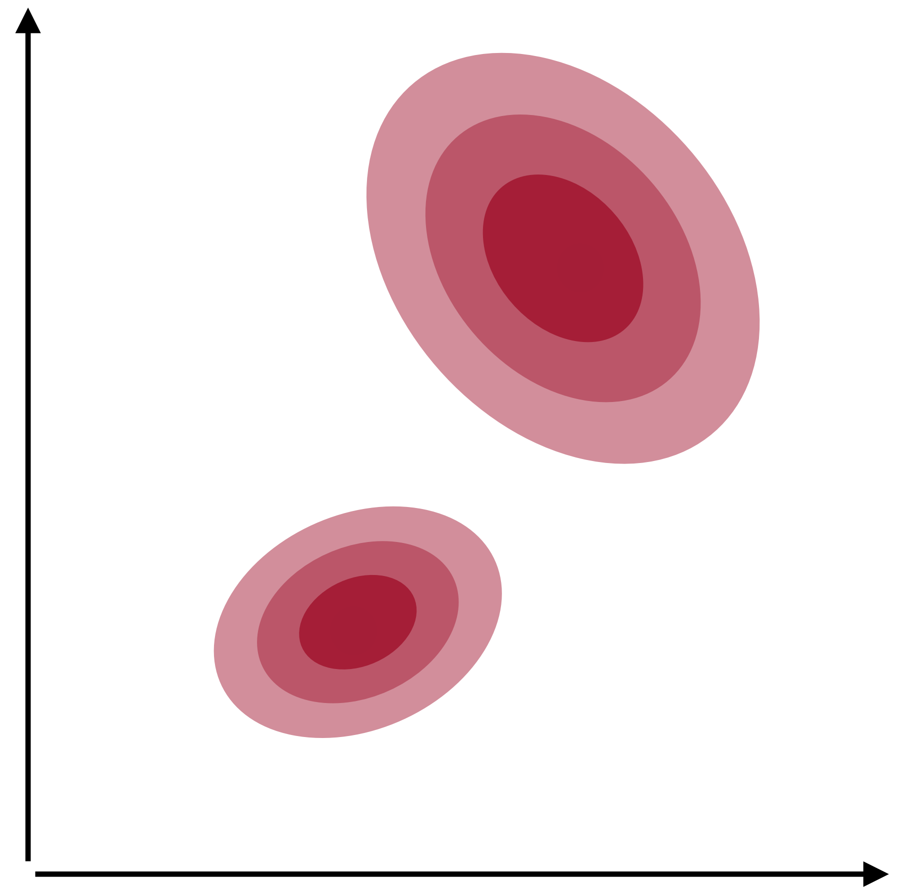


Ideal approach

- quantify uncertainty
- find all solutions
- quantify relation between solutions

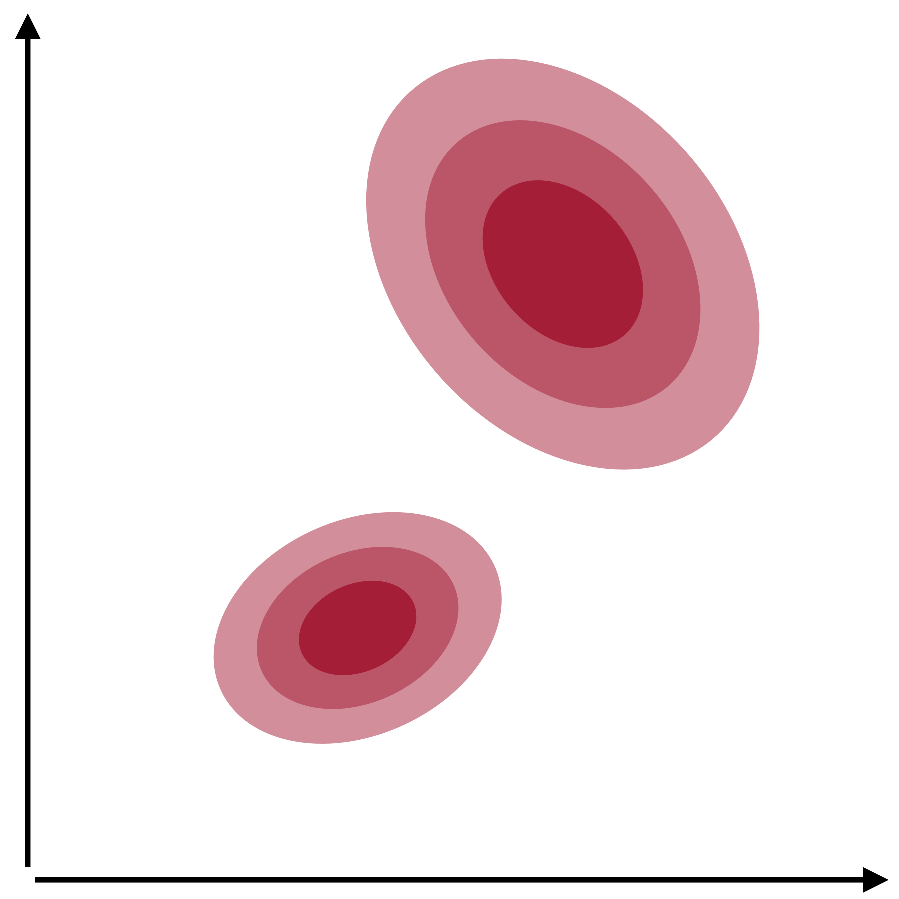
Principled approach: Bayesian inference



Thomas Bayes 1701-61

Principled approach: Bayesian inference

- data x and parameters θ are *random variables*



Thomas Bayes 1701-61

Principled approach: Bayesian inference

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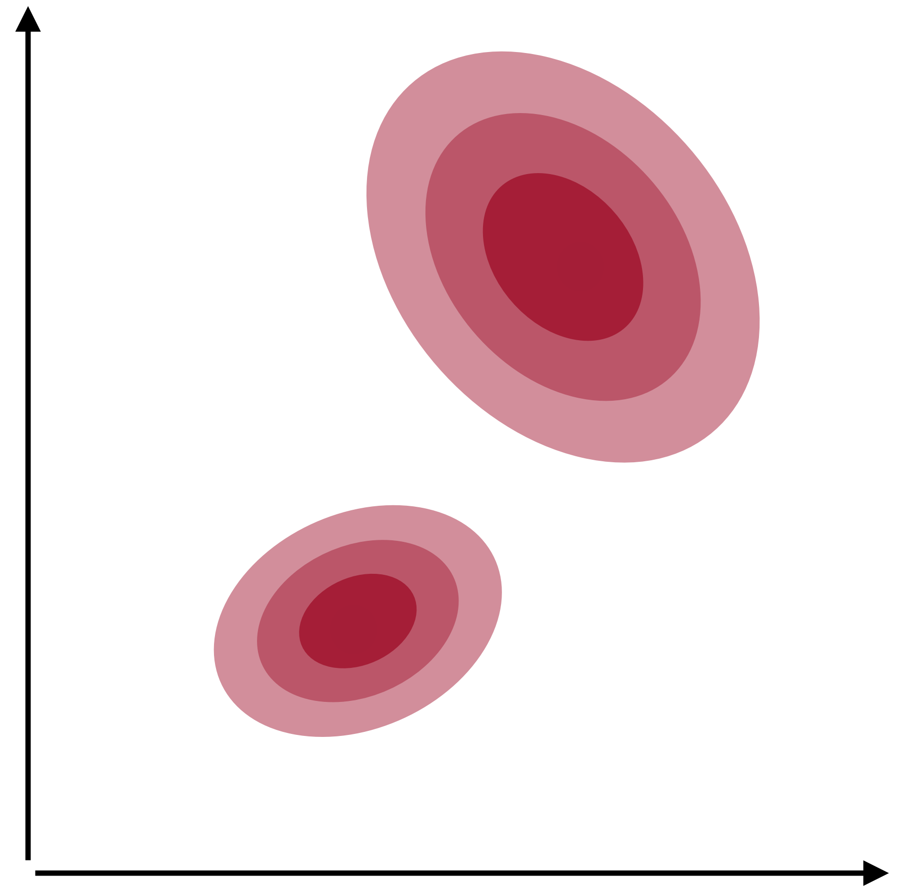
- **goal**: infer a distribution over parameters $p(\theta | x)$



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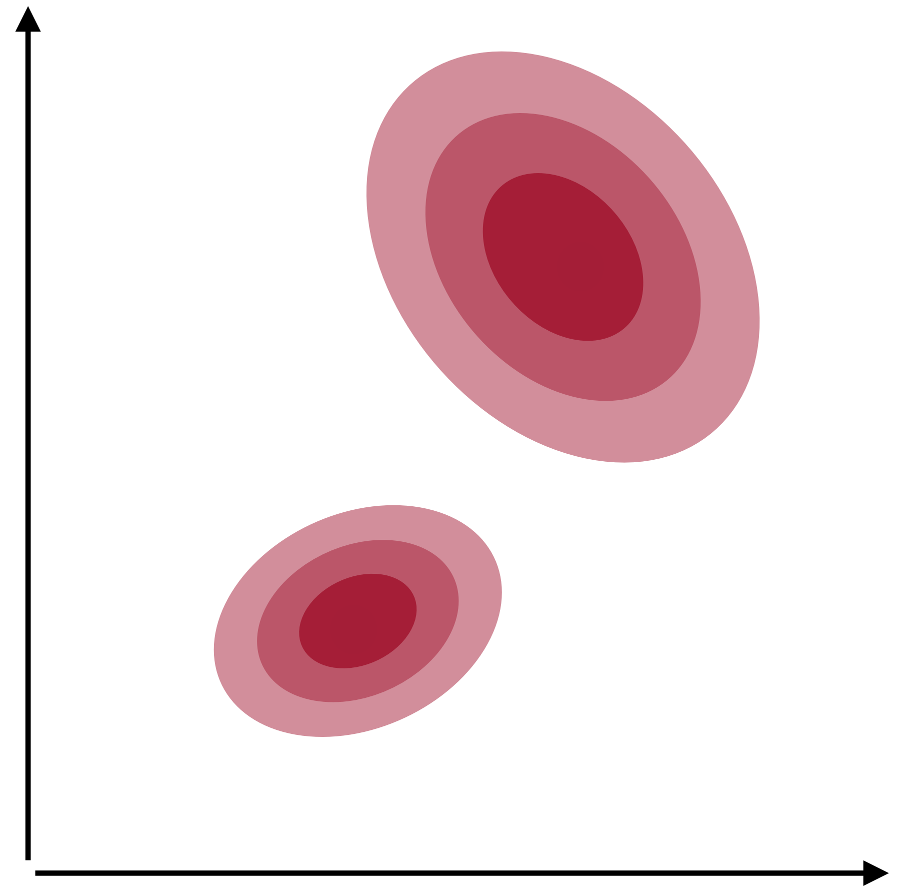

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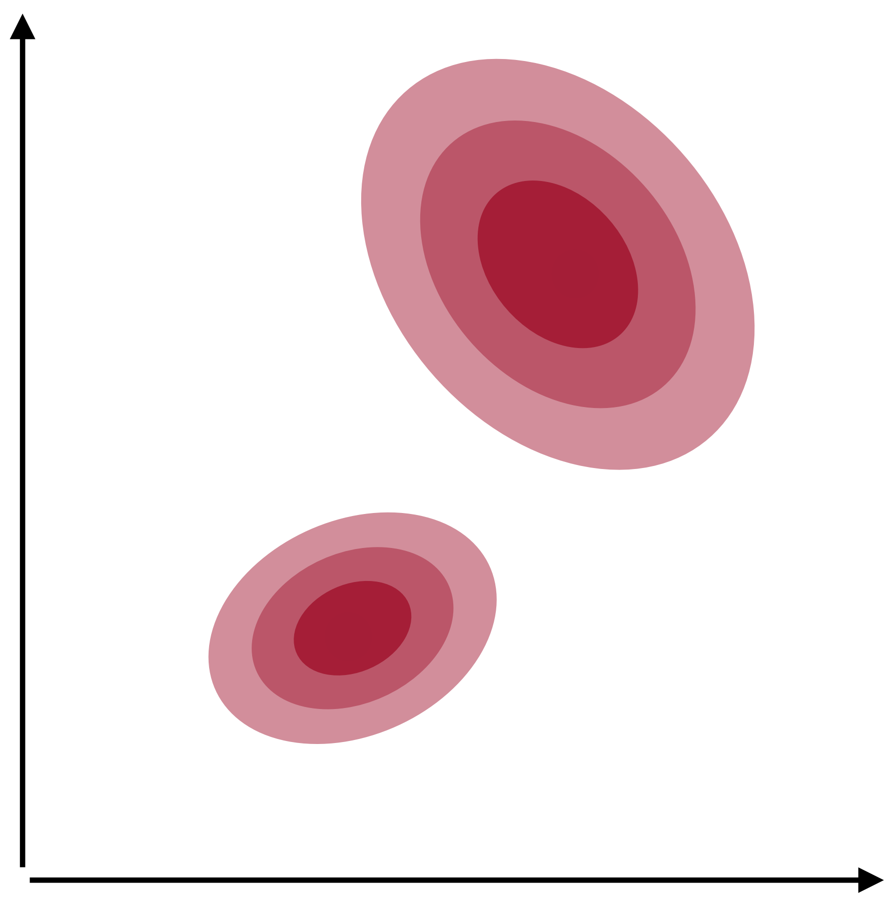
  - characterizes **all** suitable parameters
  - quantifies uncertainty



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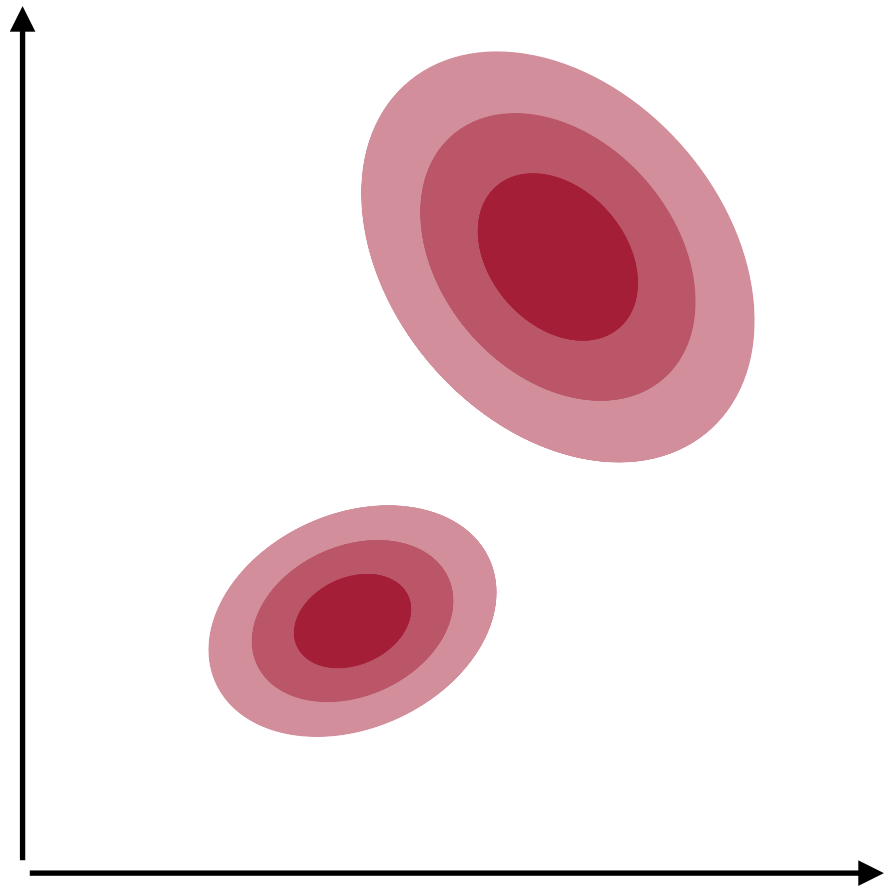

Thomas Bayes 1701-61

$$p(\theta | x) \propto p(x | \theta)\, p(\theta)$$

Principled approach: Bayesian inference

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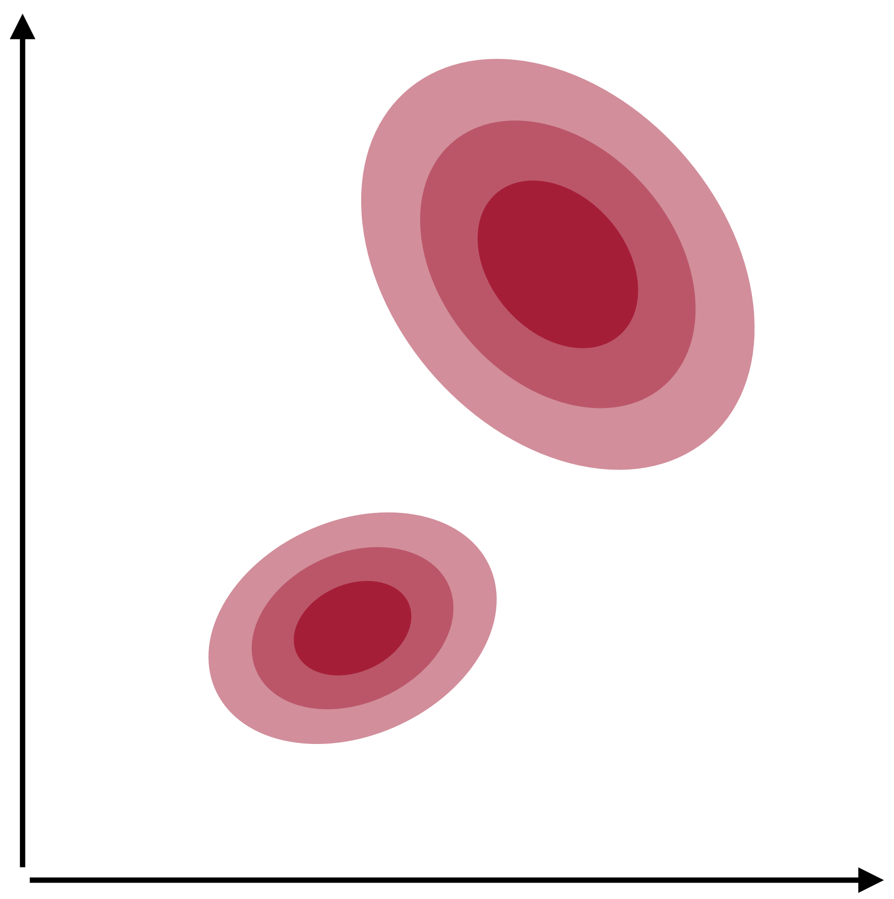

Thomas Bayes 1701-61

"posterior" → $p(\theta \mid x) \propto p(x \mid \theta)\, p(\theta)$

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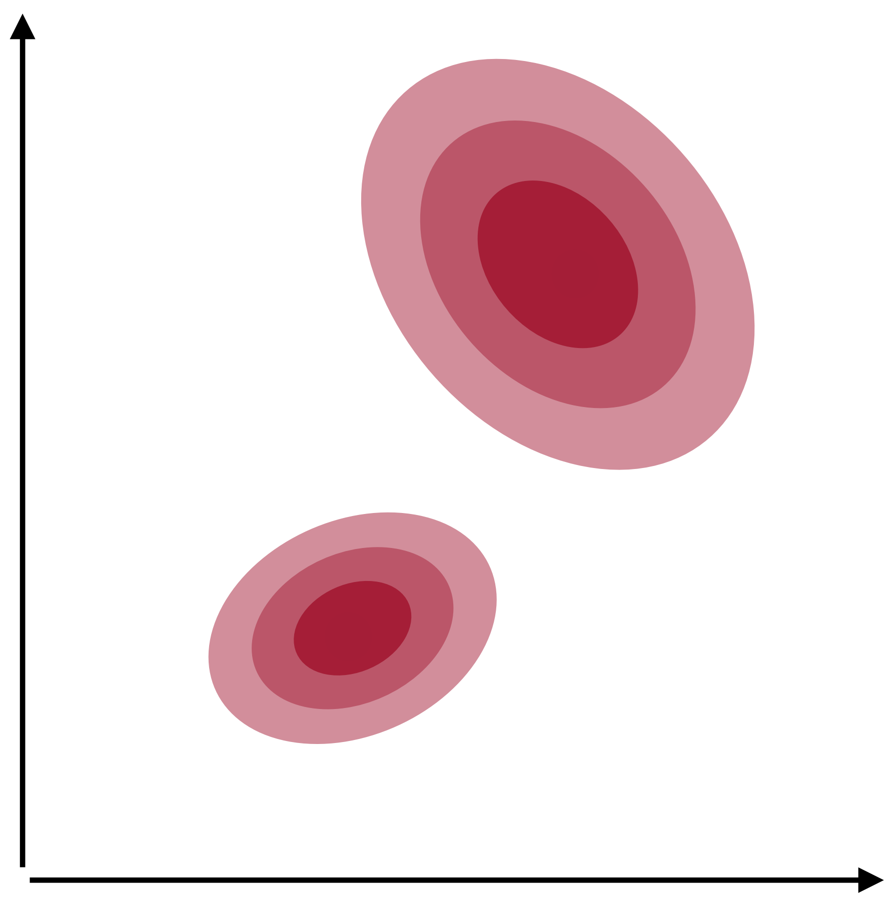

Thomas Bayes 1701-61

"prior"

"posterior" → $p(\theta | x) \propto p(x | \theta)\, p(\theta)$

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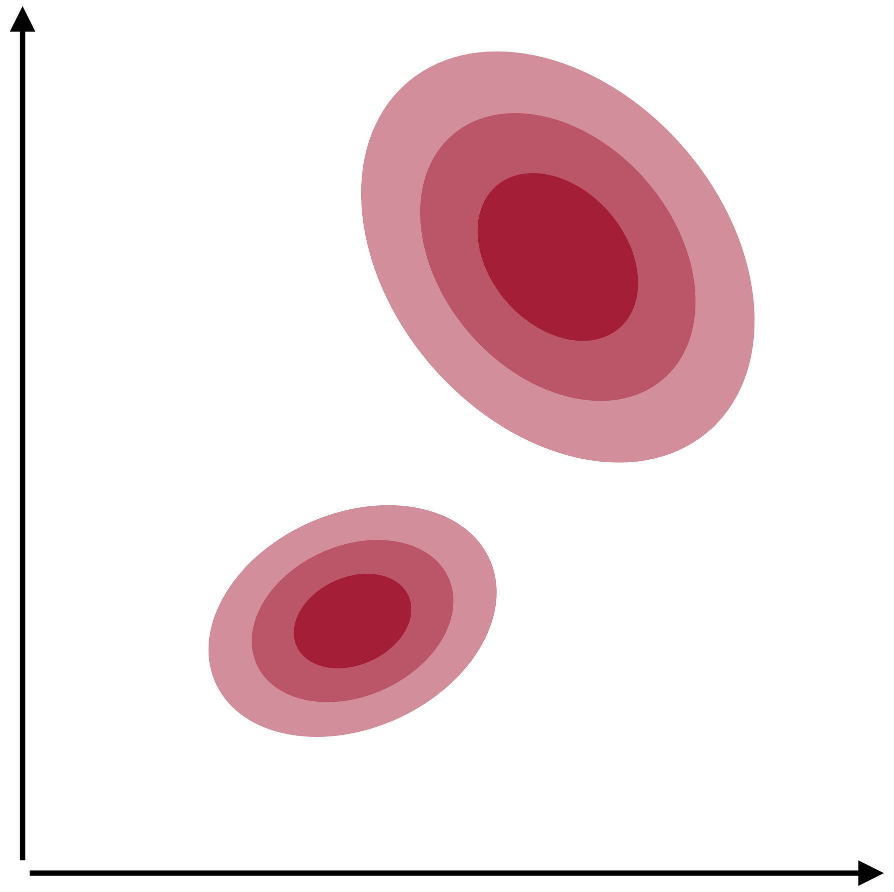
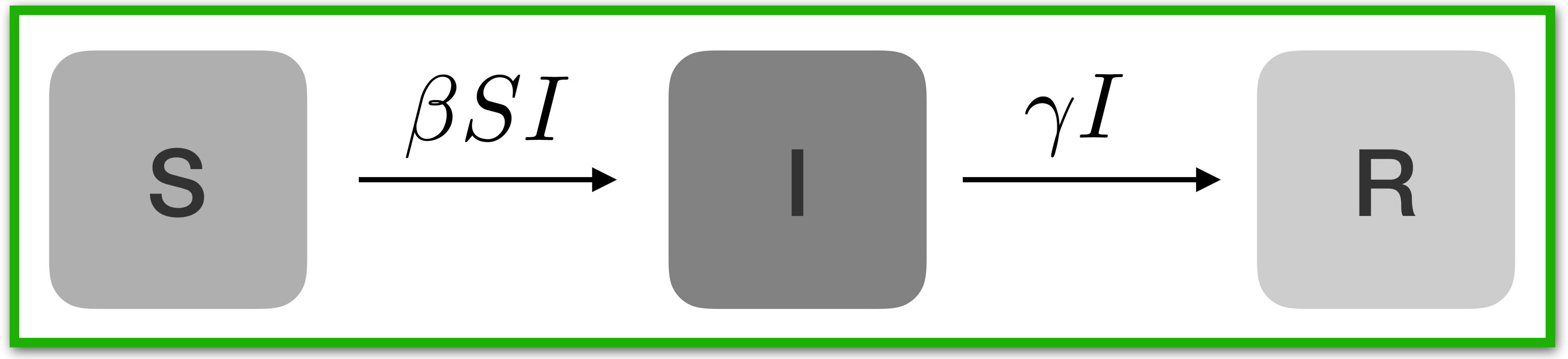


Thomas Bayes 1701-61

"likelihood" **"prior"**

"posterior" → $p(\theta | x) \propto p(x | \theta)\, p(\theta)$

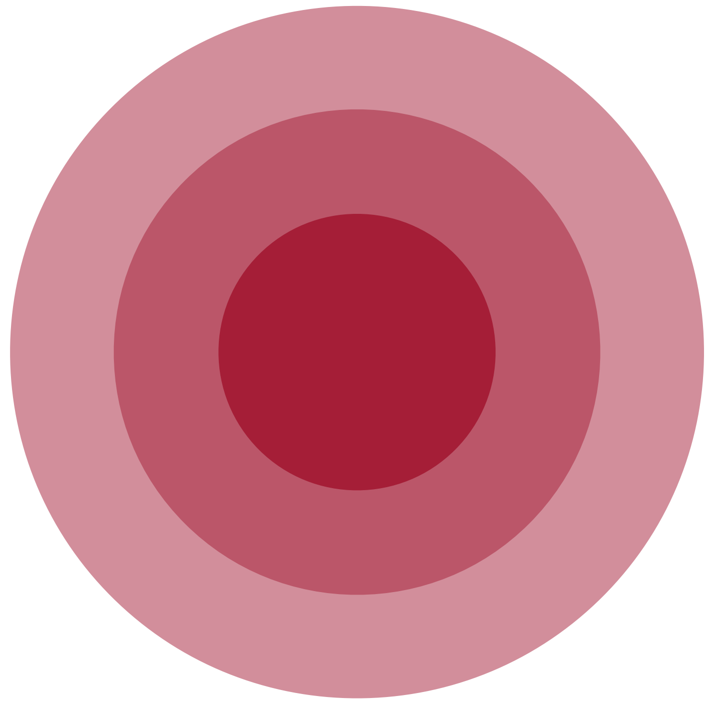
Bayesian inference for simulation-based models



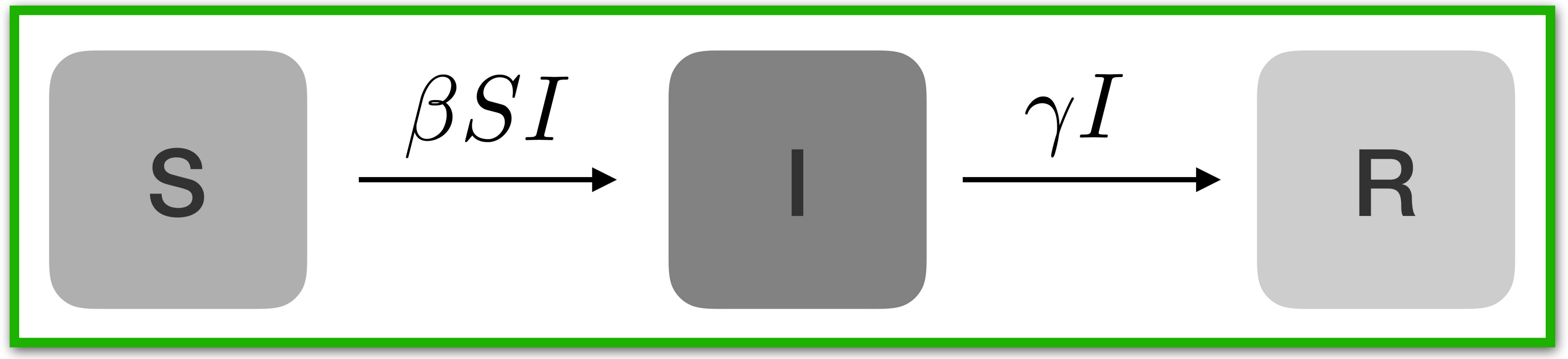
$$p(\theta | x) \propto p(x | \theta)\, p(\theta)$$

Bayesian inference for simulation-based models

parameters θ



$\theta \sim p(\theta)$



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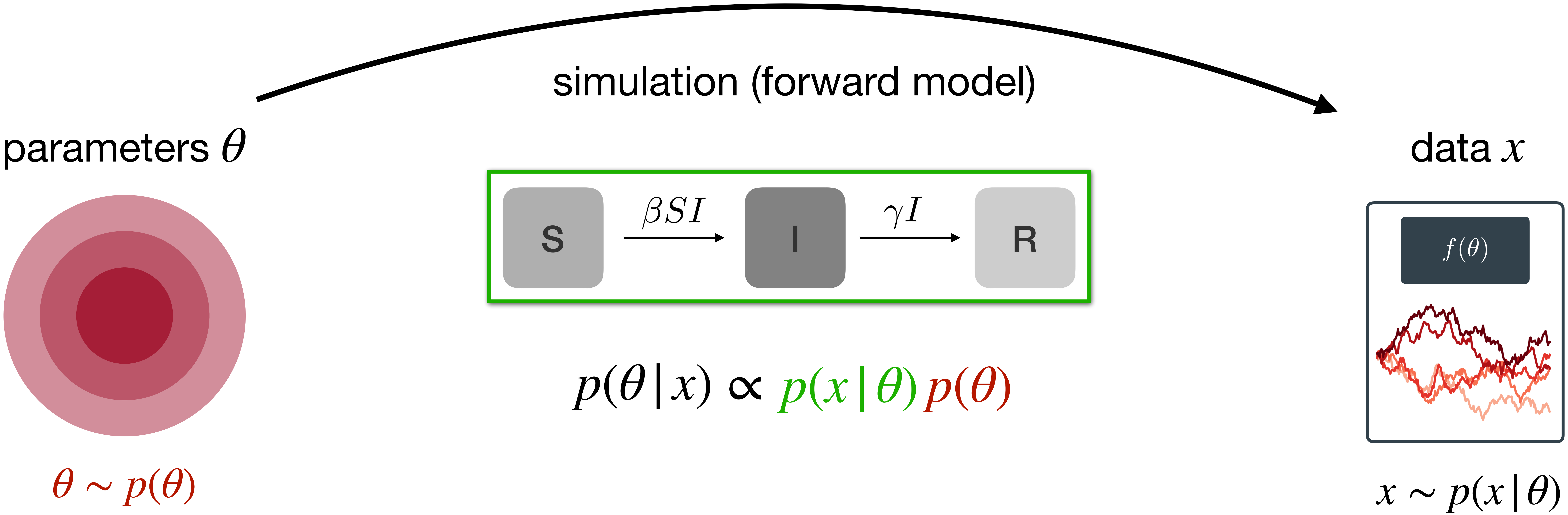

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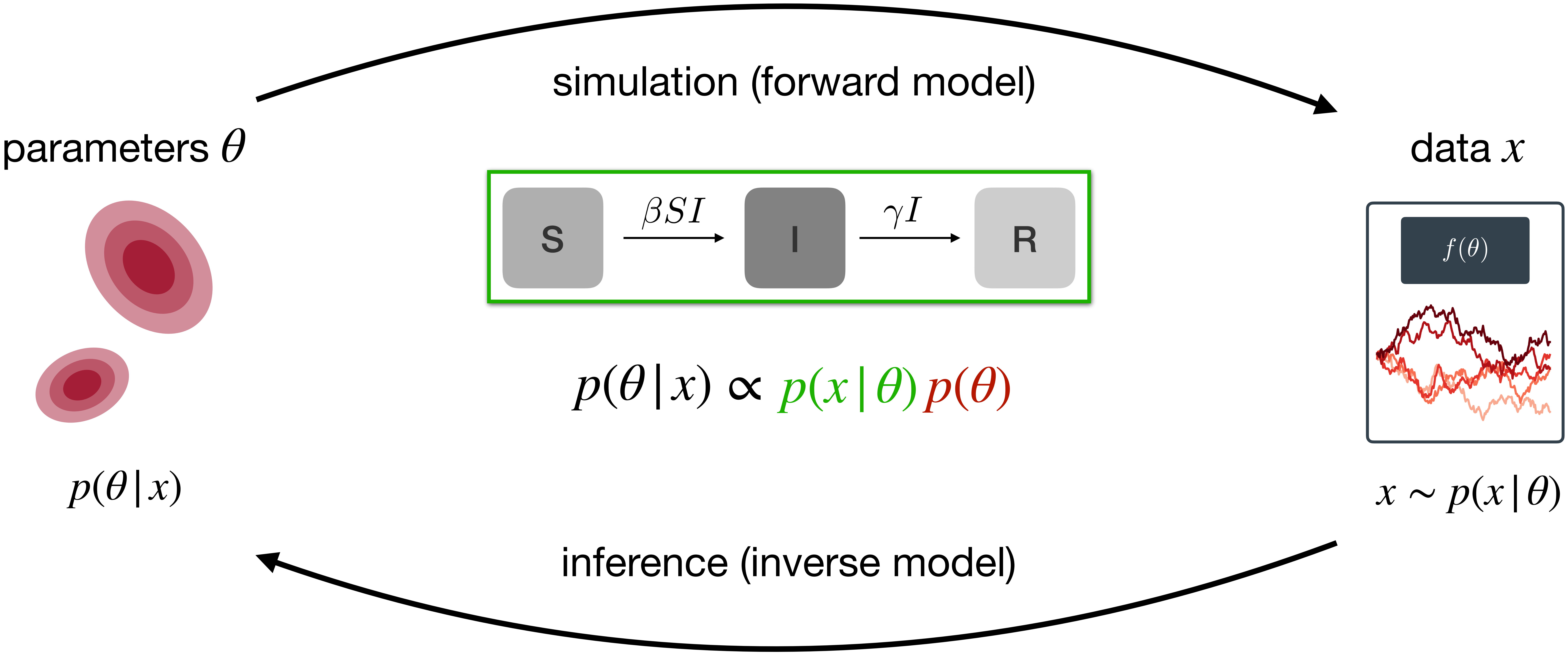
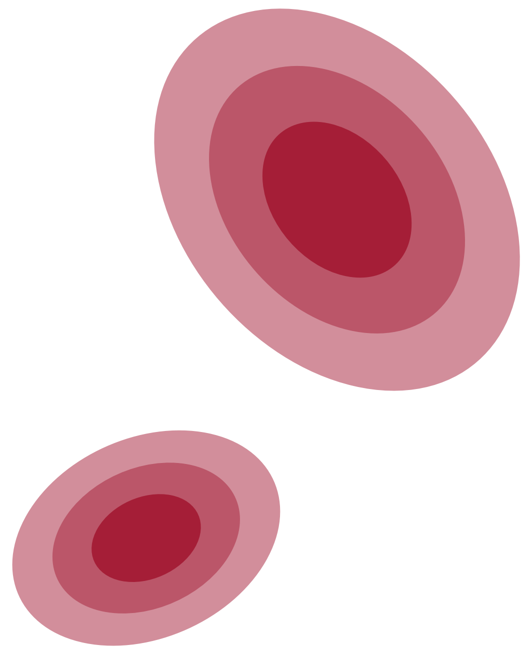
Bayesian inference for simulation-based models



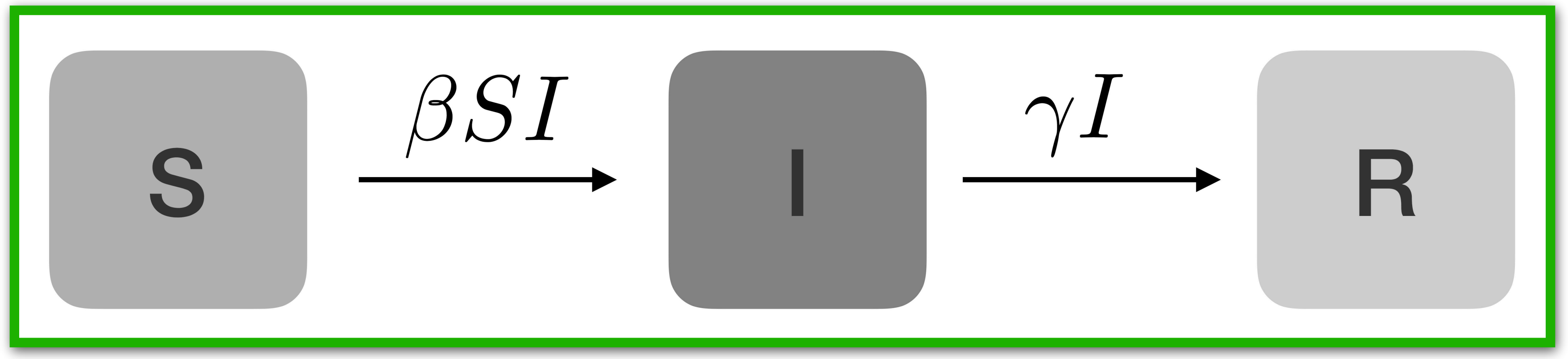
Simulation-based Bayesian inference (SBI)

forward model

parameters θ

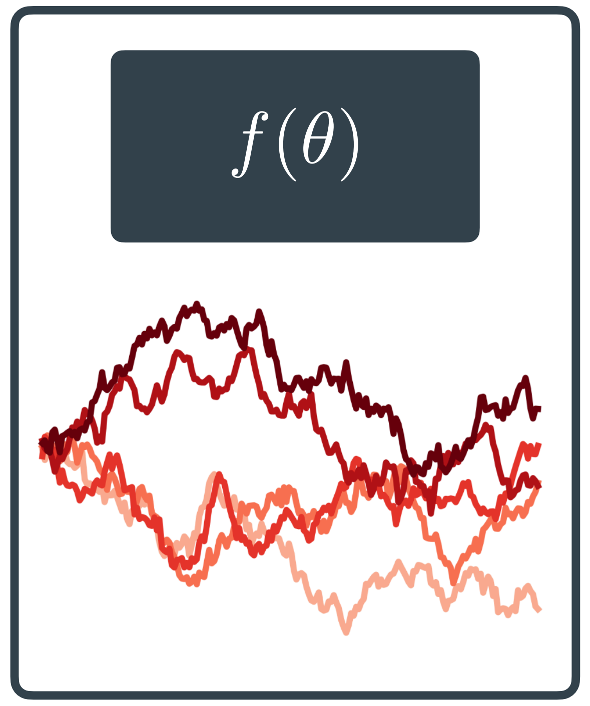


$p(\theta | x)$



$$p(\theta | x) \propto p(x | \theta)\, p(\theta)$$

data x

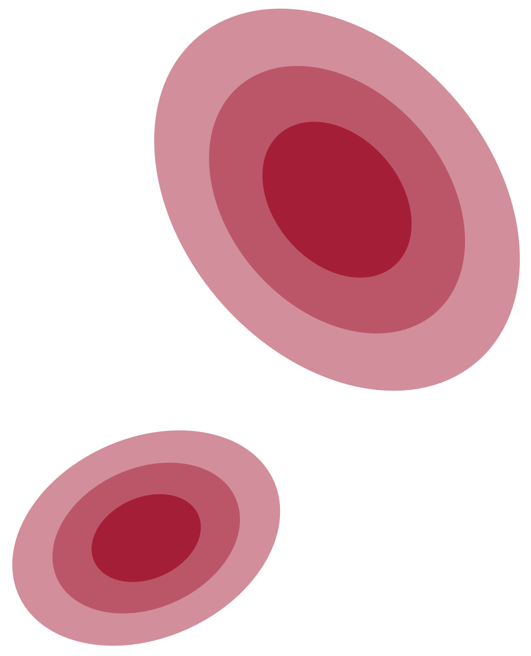


$x \sim p(x | \theta)$

Simulation-based Bayesian inference (SBI)

forward model

parameters θ



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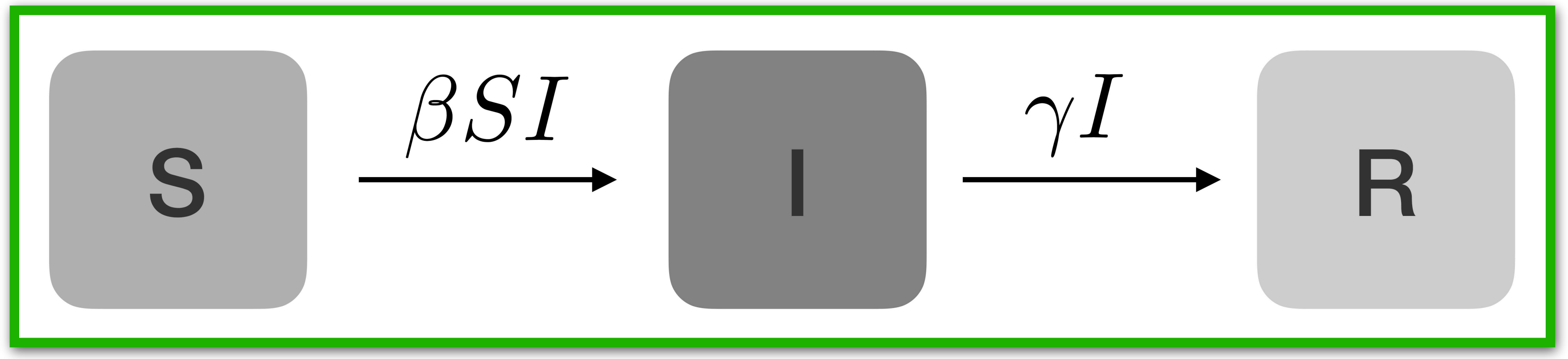

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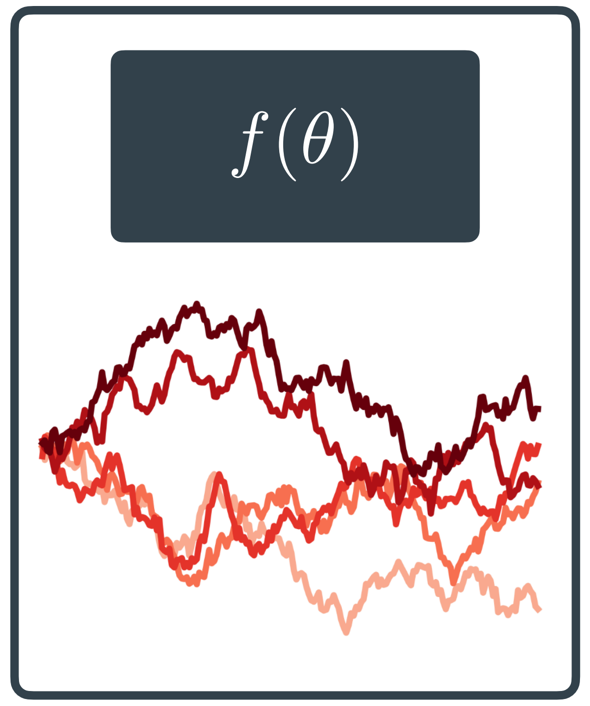

$x \sim p(x | \theta)$

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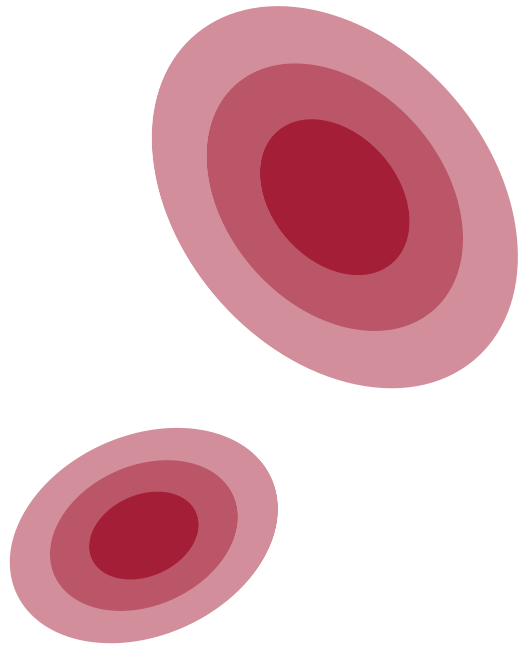

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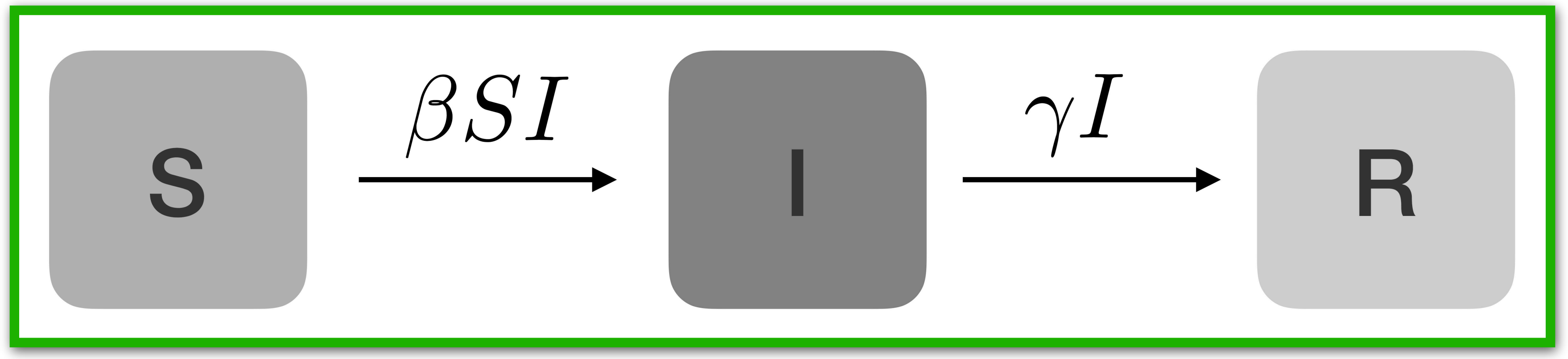

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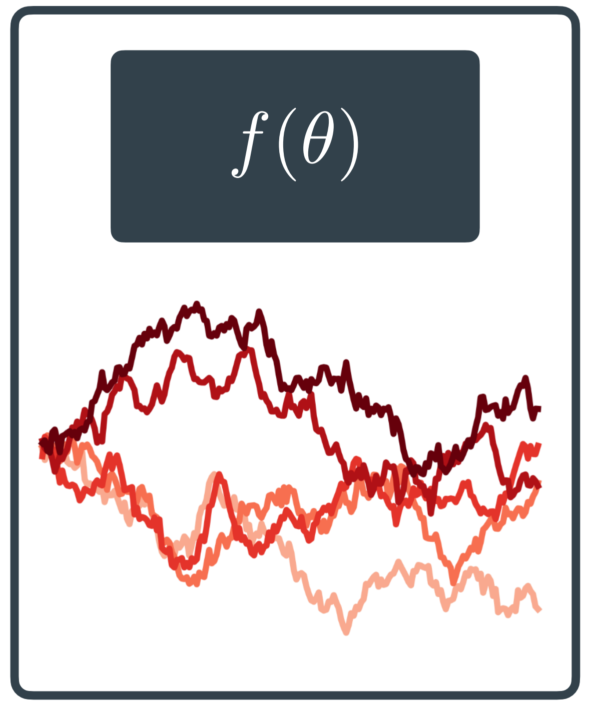

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Simulation-based Bayesian inference (SBI)

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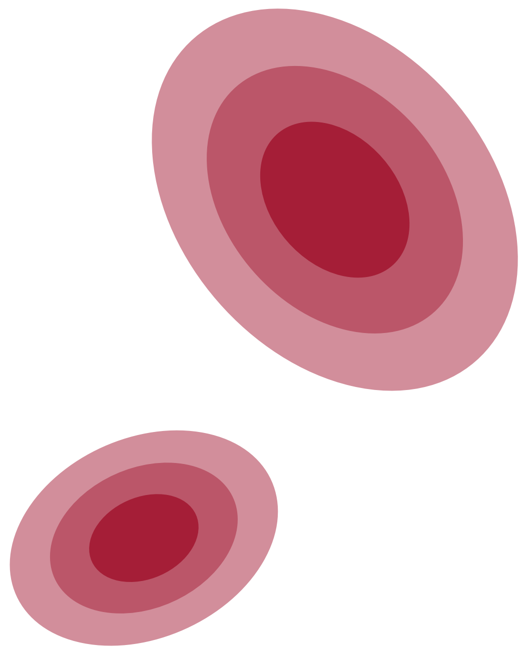
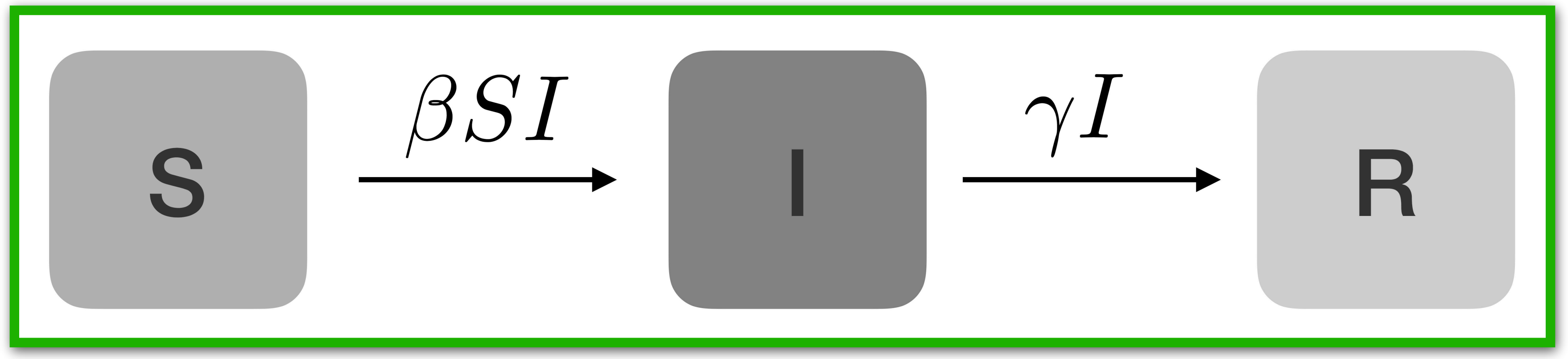


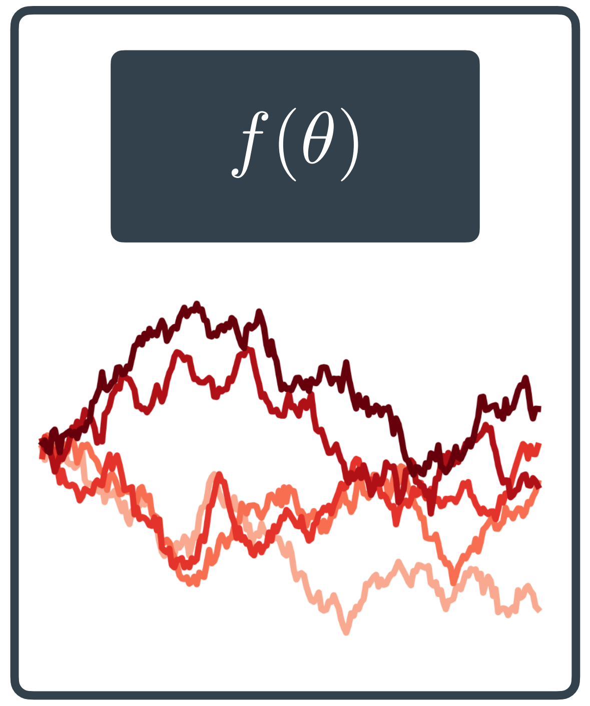
$p(\theta | x)$



$$p(\theta | x) \propto p(x | \theta) p(\theta)$$

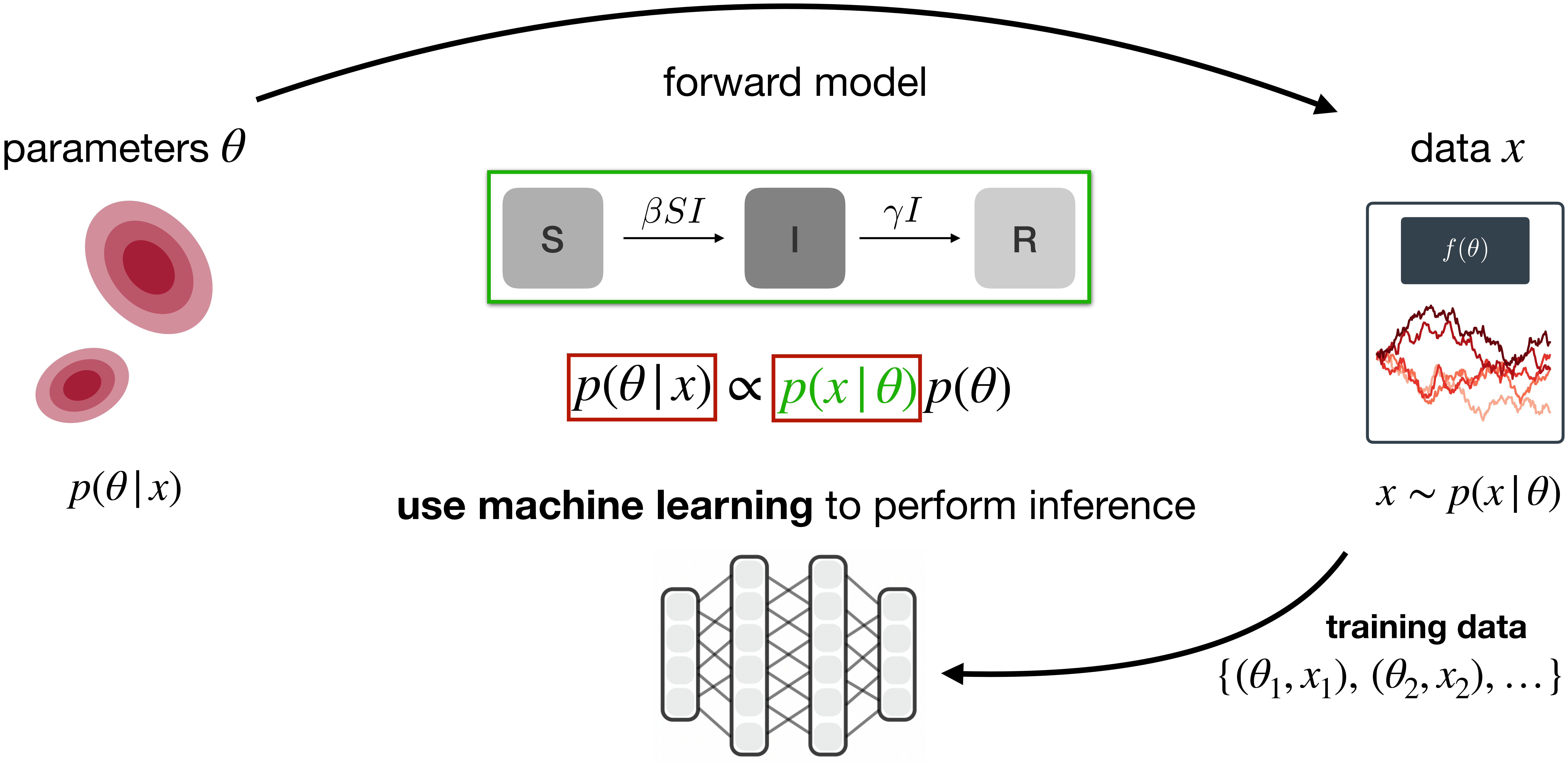
use machine learning to perform inference

data x



$x \sim p(x | \theta)$

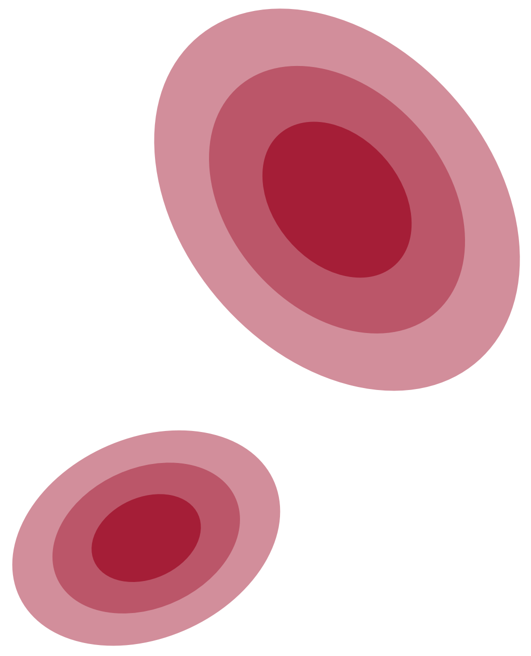
Simulation-based Bayesian inference (SBI)



Simulation-based Bayesian inference (SBI)

forward model

parameters θ

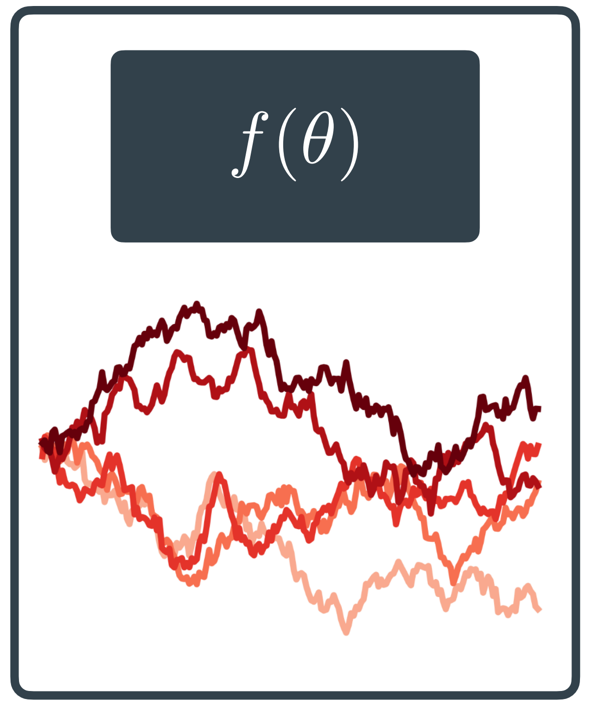


$p(\theta | x)$

S $\xrightarrow{\beta SI}$ I $\xrightarrow{\gamma I}$ R

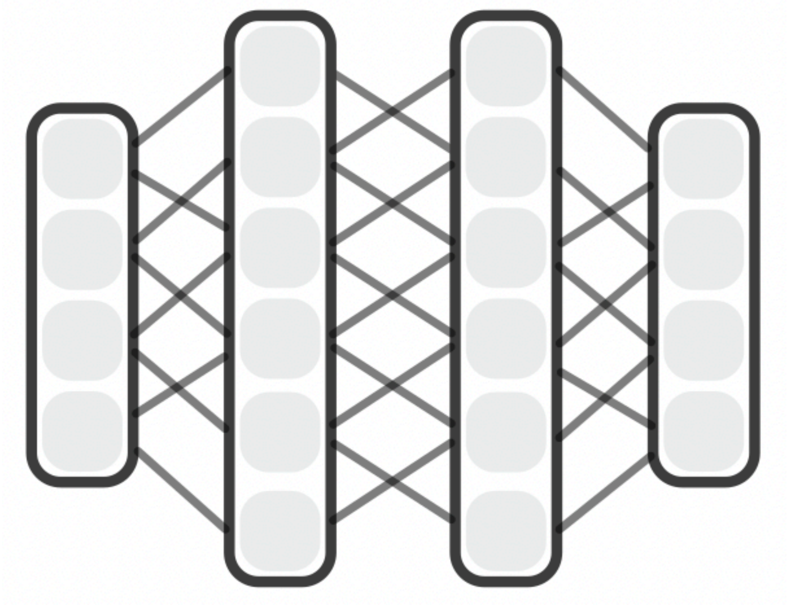
$$p(\theta | x) \propto p(x | \theta) p(\theta)$$

data x



$x \sim p(x | \theta)$

use machine learning to perform inference



training data

$\{(\theta_1, x_1), (\theta_2, x_2), \ldots\}$

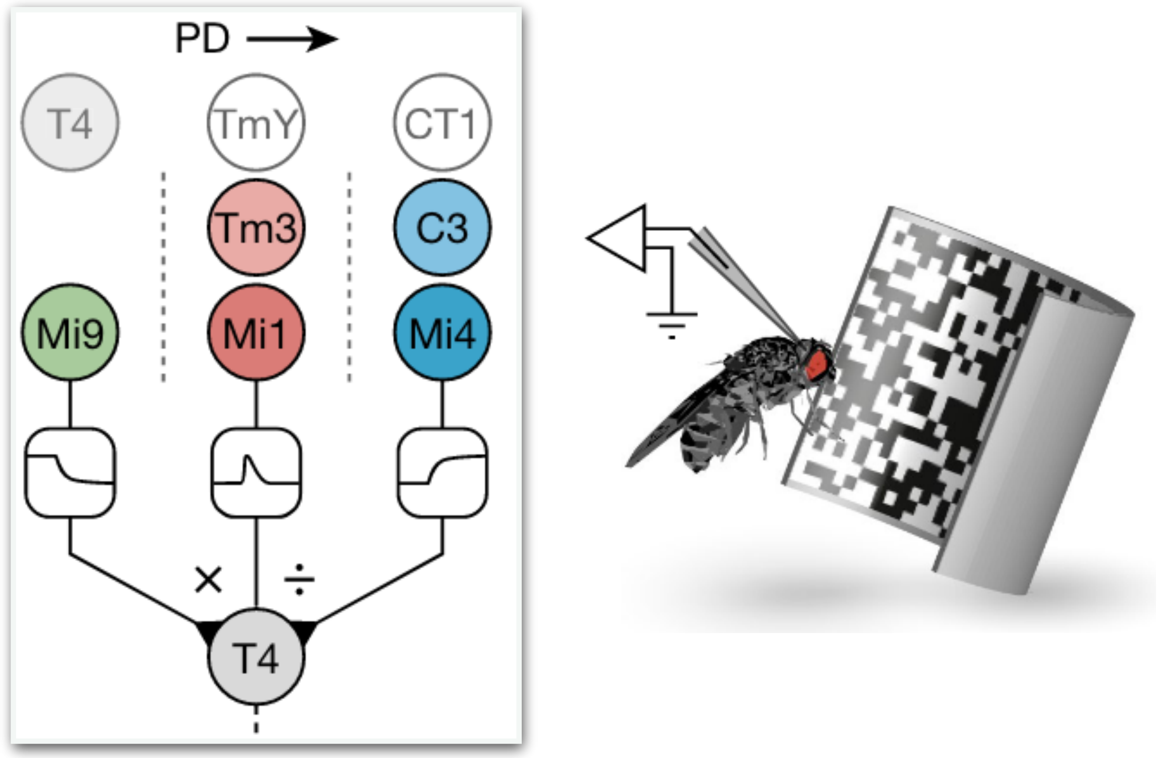
SBI in neuroscience

- Recent examples:

Groschner et al. 2022; Hashemi et al. 2023

SBI in neuroscience

- Recent examples:



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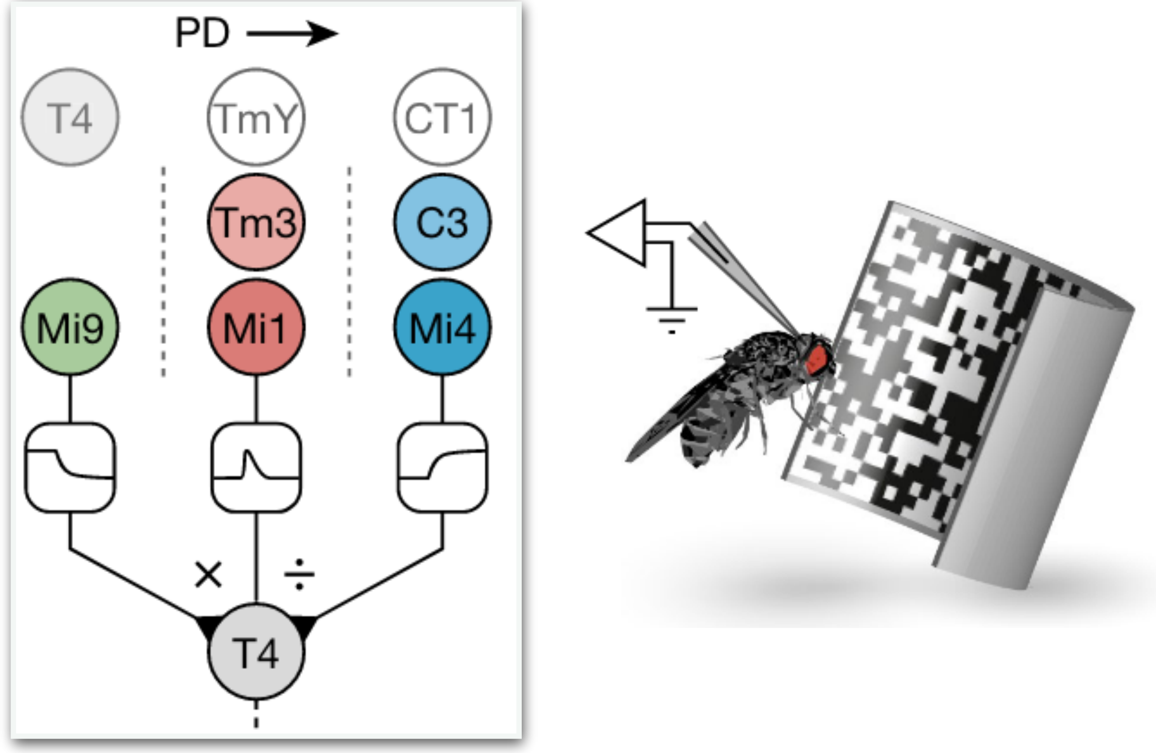
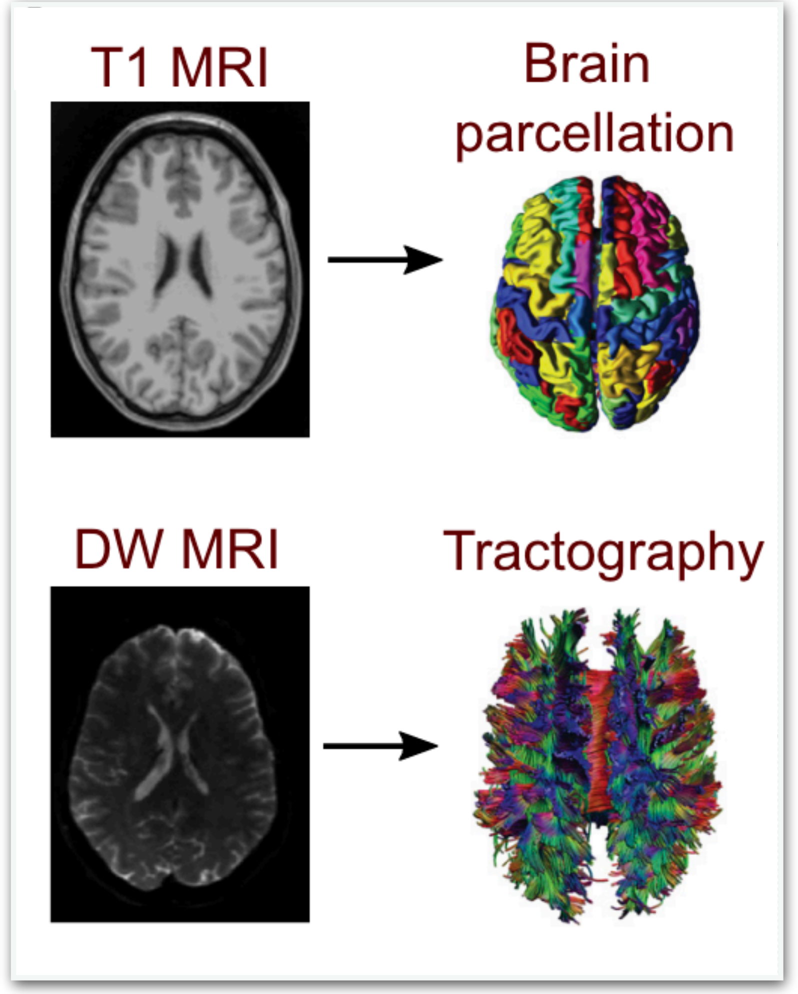
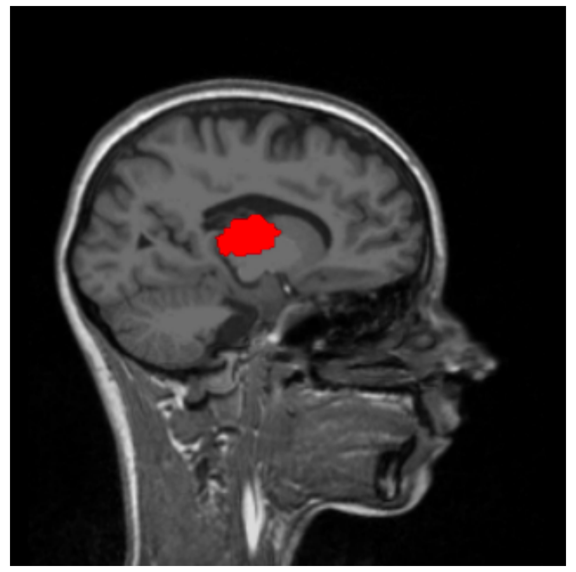
SBI in neuroscience

- Recent examples:







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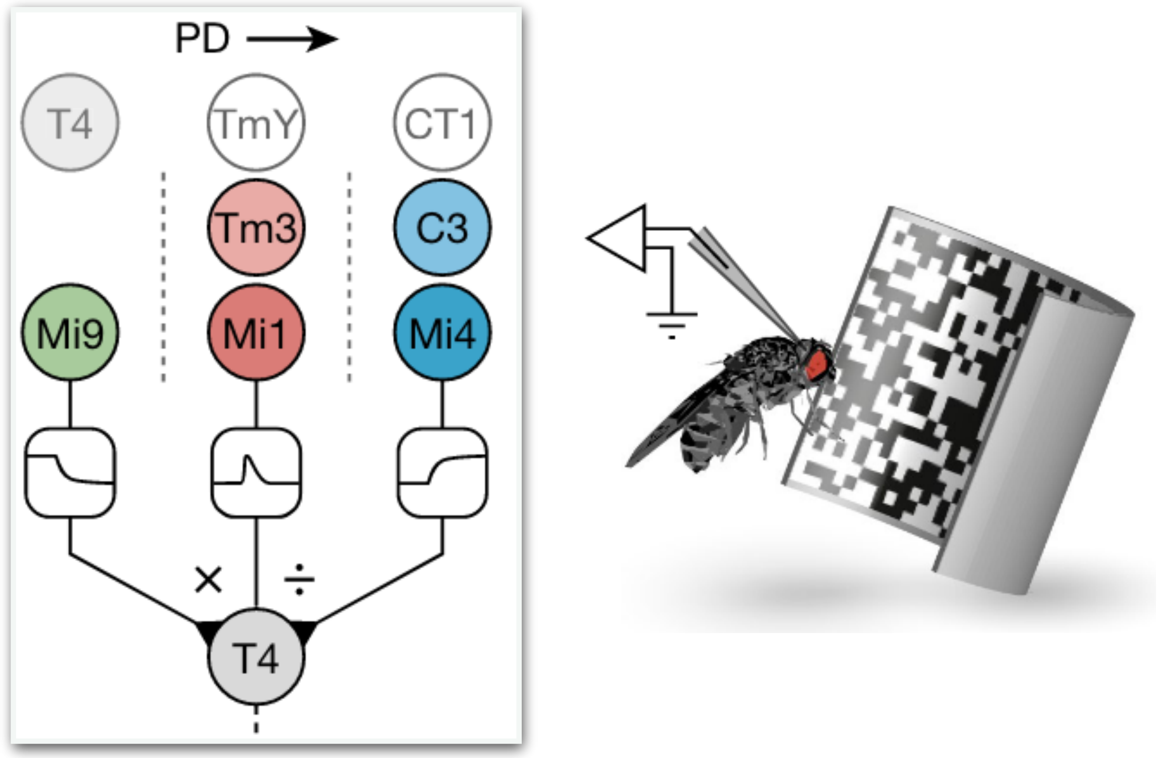

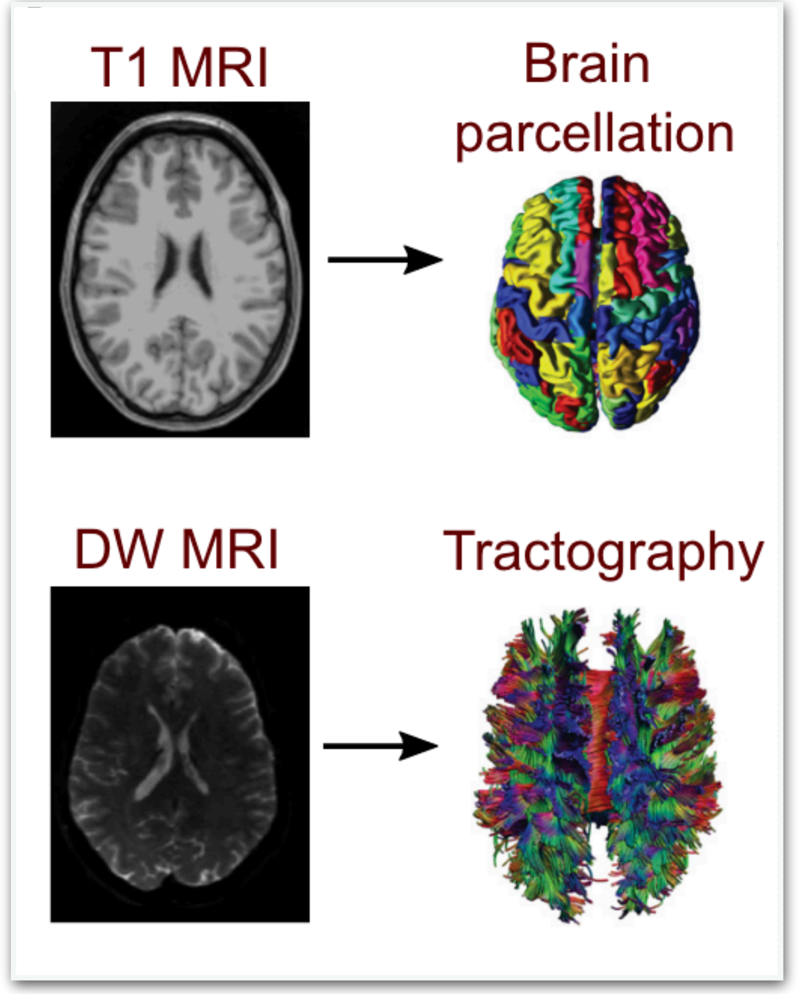

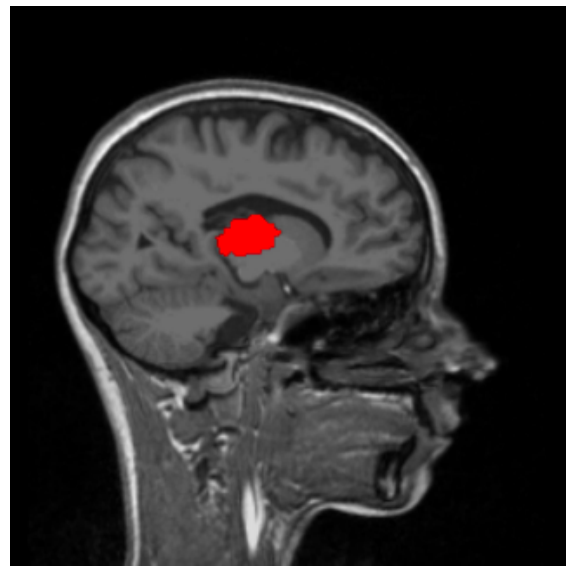

- Challenges and Opportunities:

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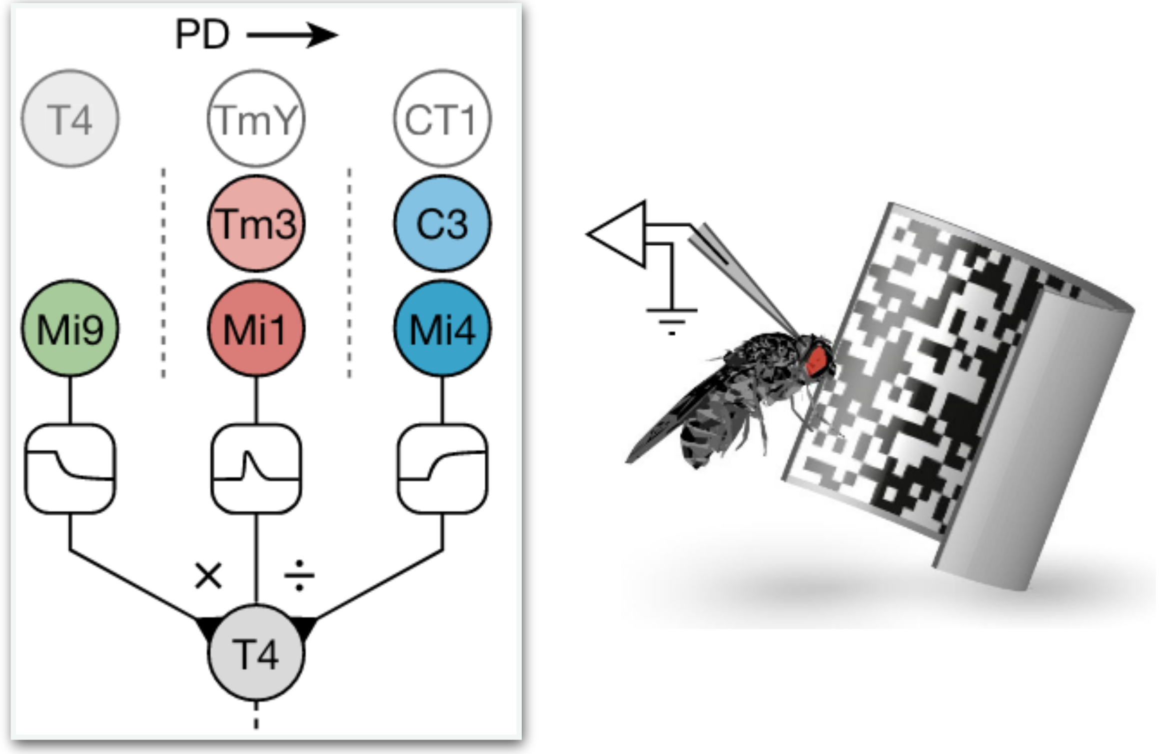
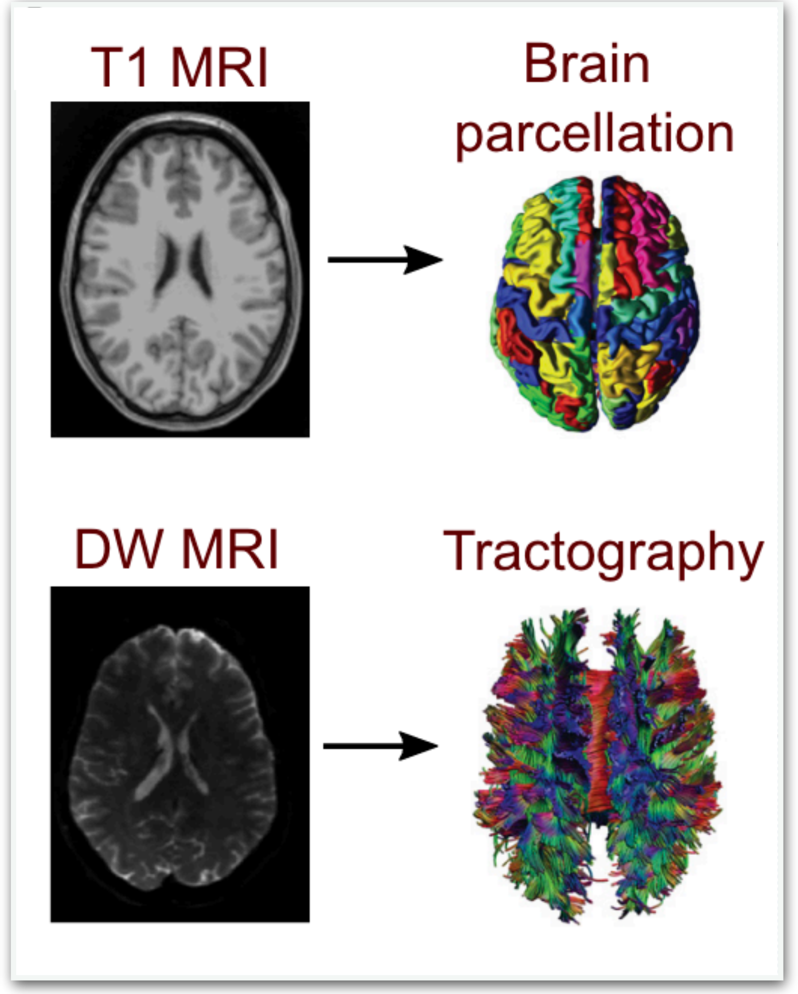
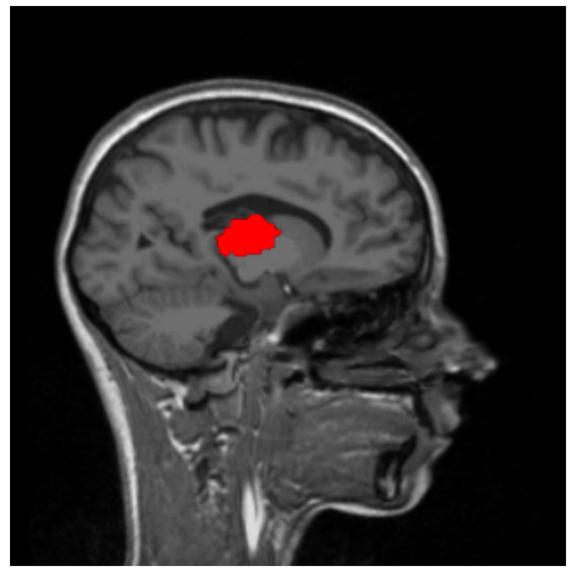
SBI in neuroscience

- Recent examples:







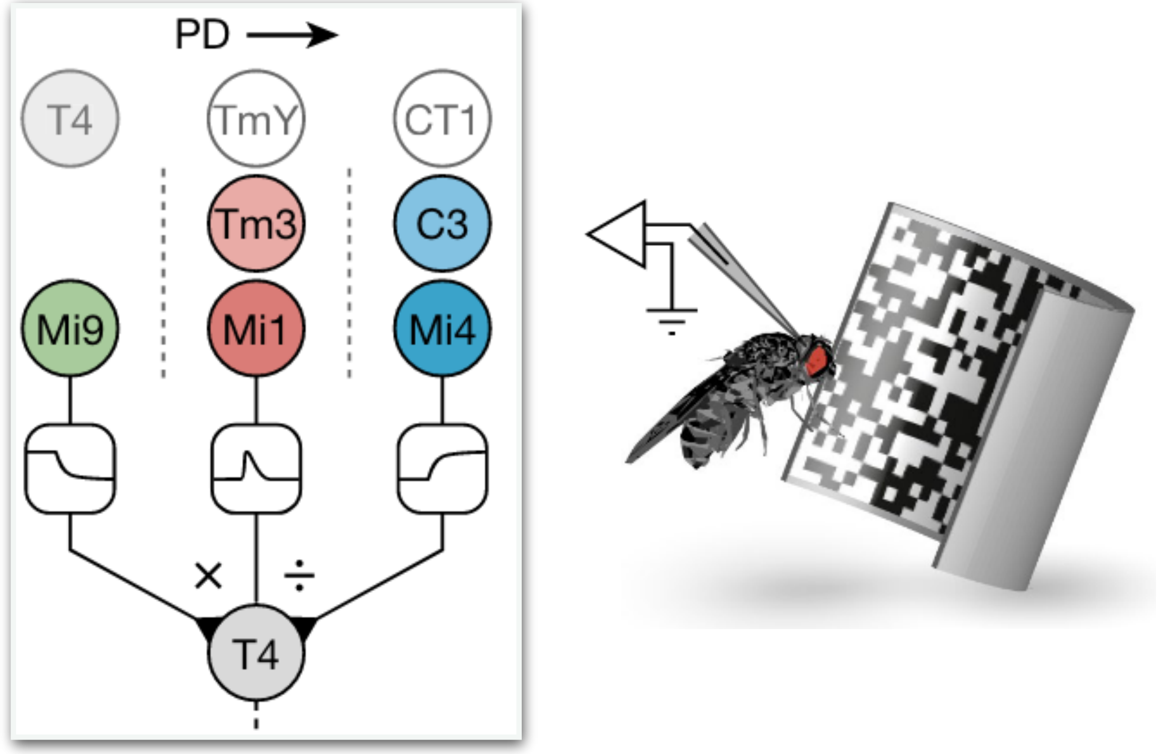
- Challenges and Opportunities:

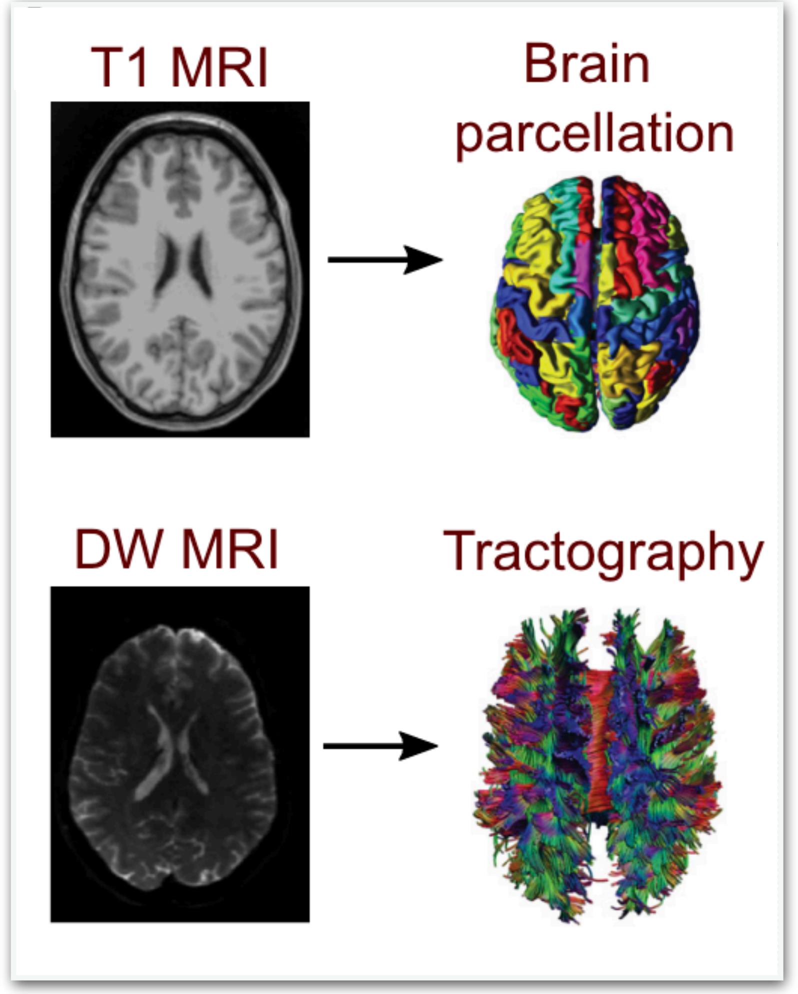
    1. Current SBI methods struggle with some models

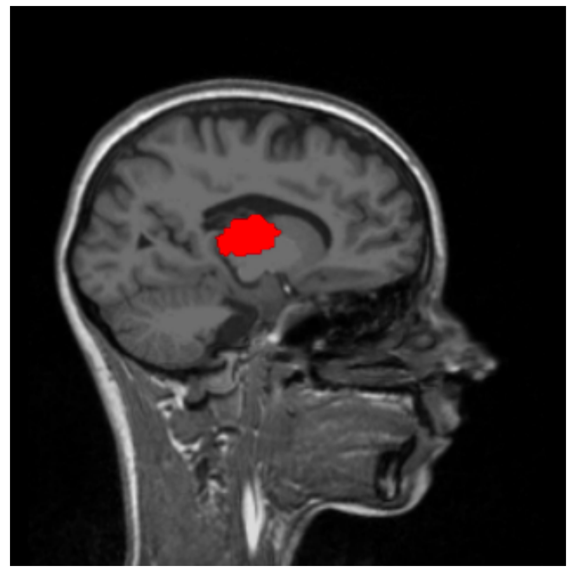
Groschner et al. 2022; Hashemi et al. 2023

SBI in neuroscience

- Recent examples:





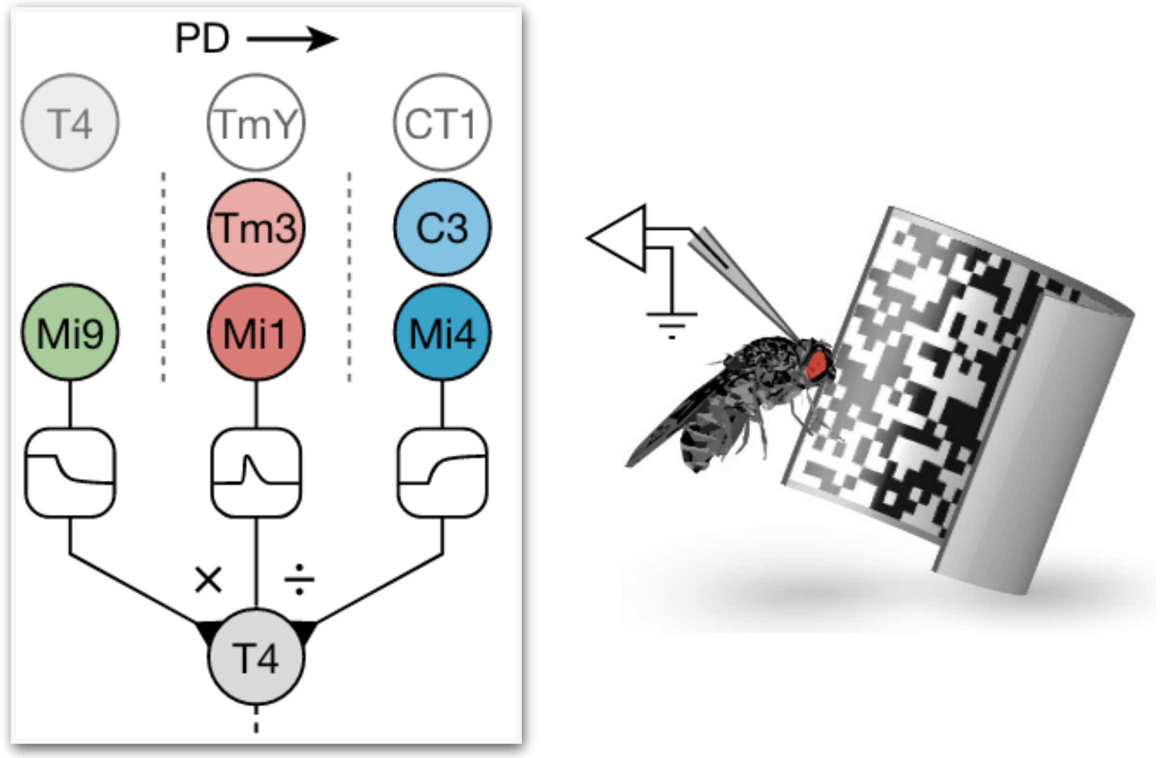


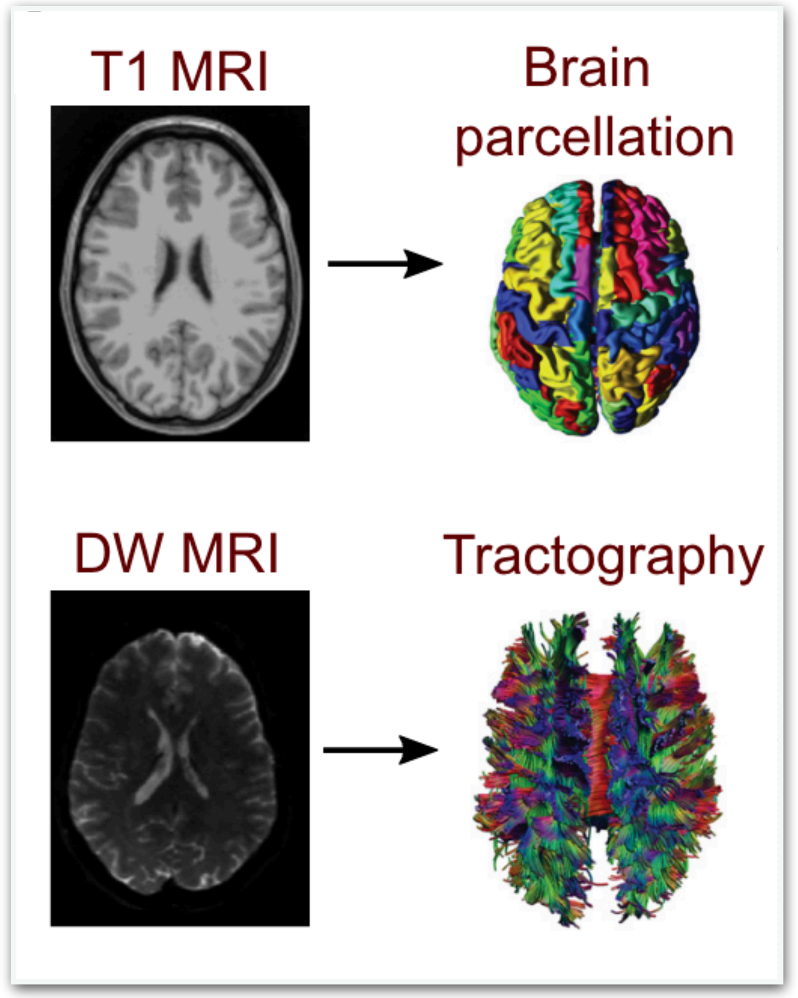
- Challenges and Opportunities:
    1. Current SBI methods struggle with some models
    2. Unexplored subfields in neuroscience where SBI can be useful

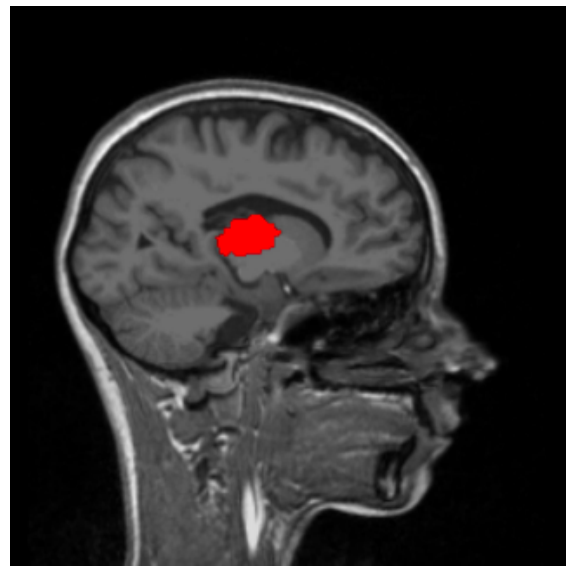
Groschner et al. 2022; Hashemi et al. 2023

SBI in neuroscience

- Recent examples:







- Challenges and Opportunities:

    1. Current SBI methods struggle with some models
    2. Unexplored subfields in neuroscience where SBI can be useful
    3. Accessible software tools and guidelines

Groschner et al. 2022; Hashemi et al. 2023

Advancing Methods and Applicability of SBI in neuroscience

Advancing Methods and Applicability of SBI in neuroscience

1. A new SBI method for **decision-making research**

Advancing Methods and Applicability of SBI in neuroscience

1. A new SBI method for **decision-making research**

2. How to apply SBI in **Connectomics**

Advancing Methods and Applicability of SBI in neuroscience

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Advancing Methods and Applicability of SBI in neuroscience

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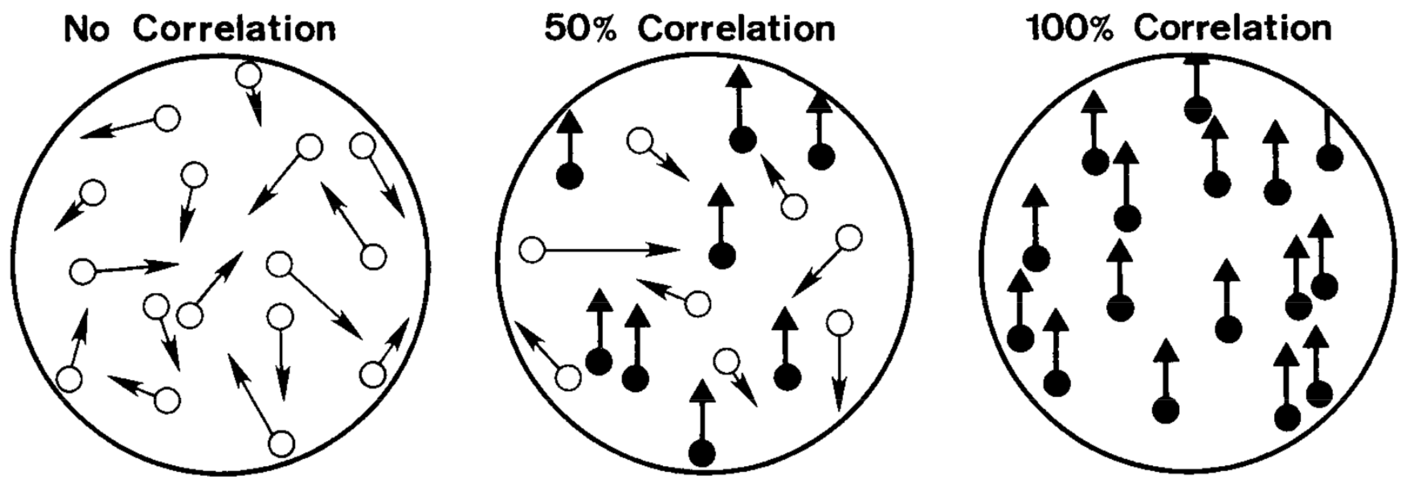
Studying decision-making in the brain

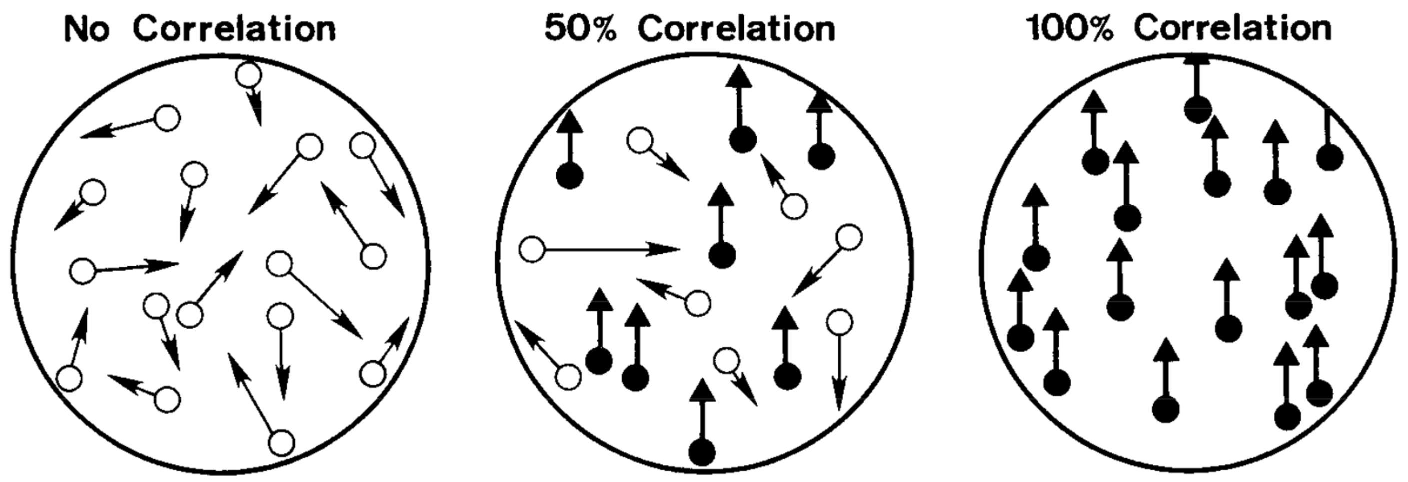
- Start simple: perceptual decision-making



Newsome & Pare, 1988; Roitmann & Shadlen, 2002; Sanchez 2014

Studying decision-making in the brain

- Start simple: perceptual decision-making
- Random dot motion task



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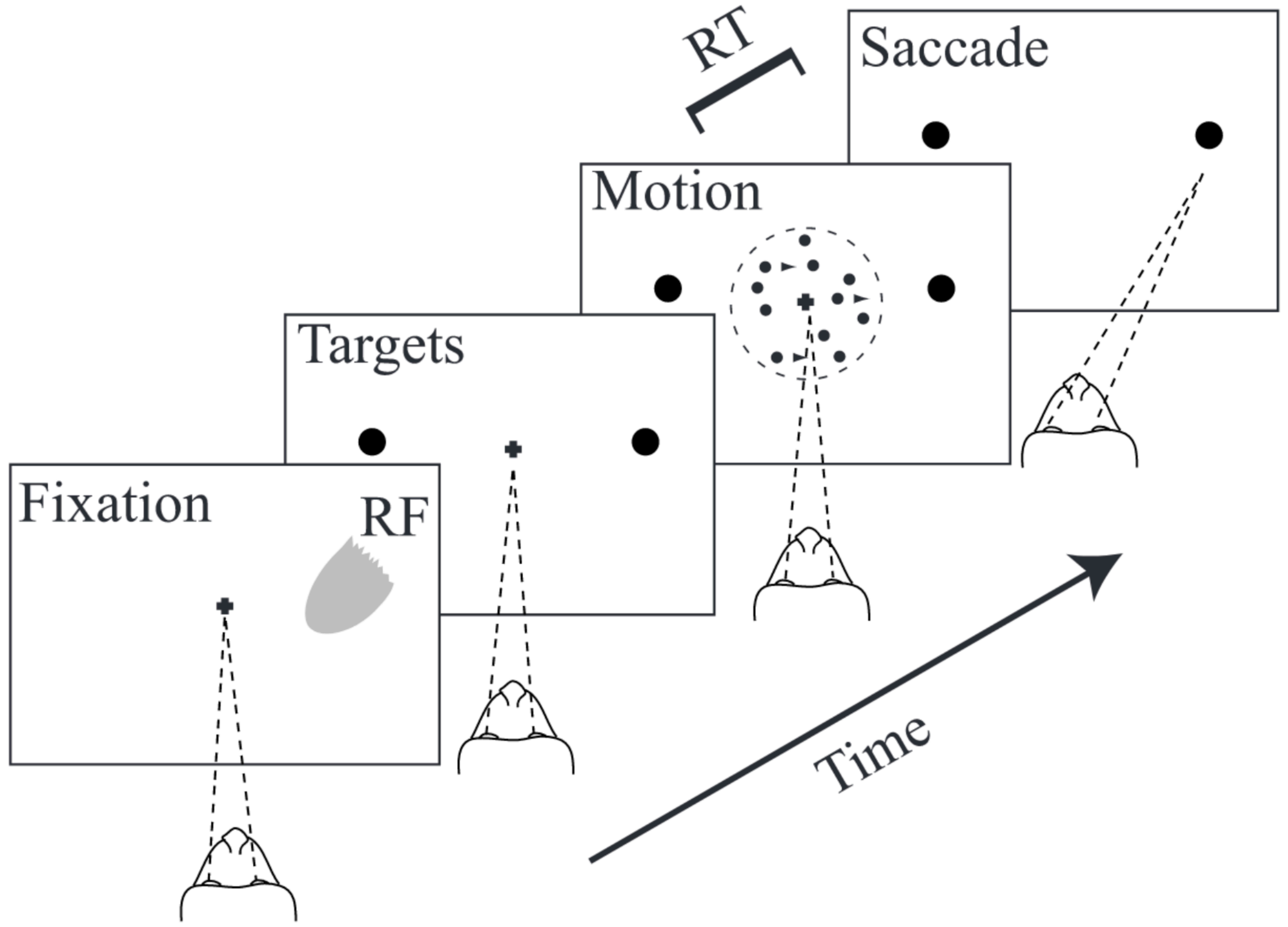

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Studying decision-making in the brain

- Start simple: perceptual decision-making
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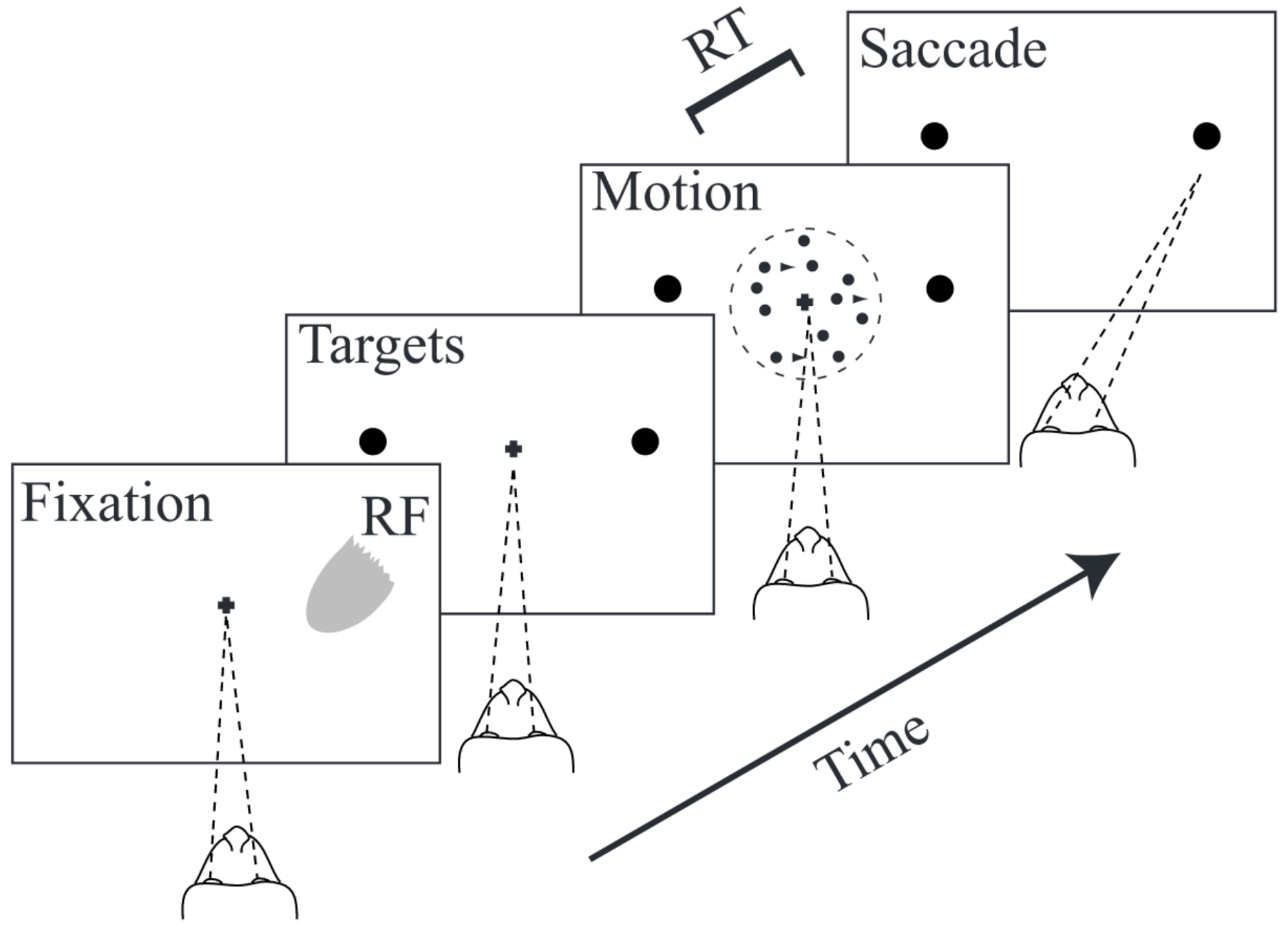
- Behavioral data:



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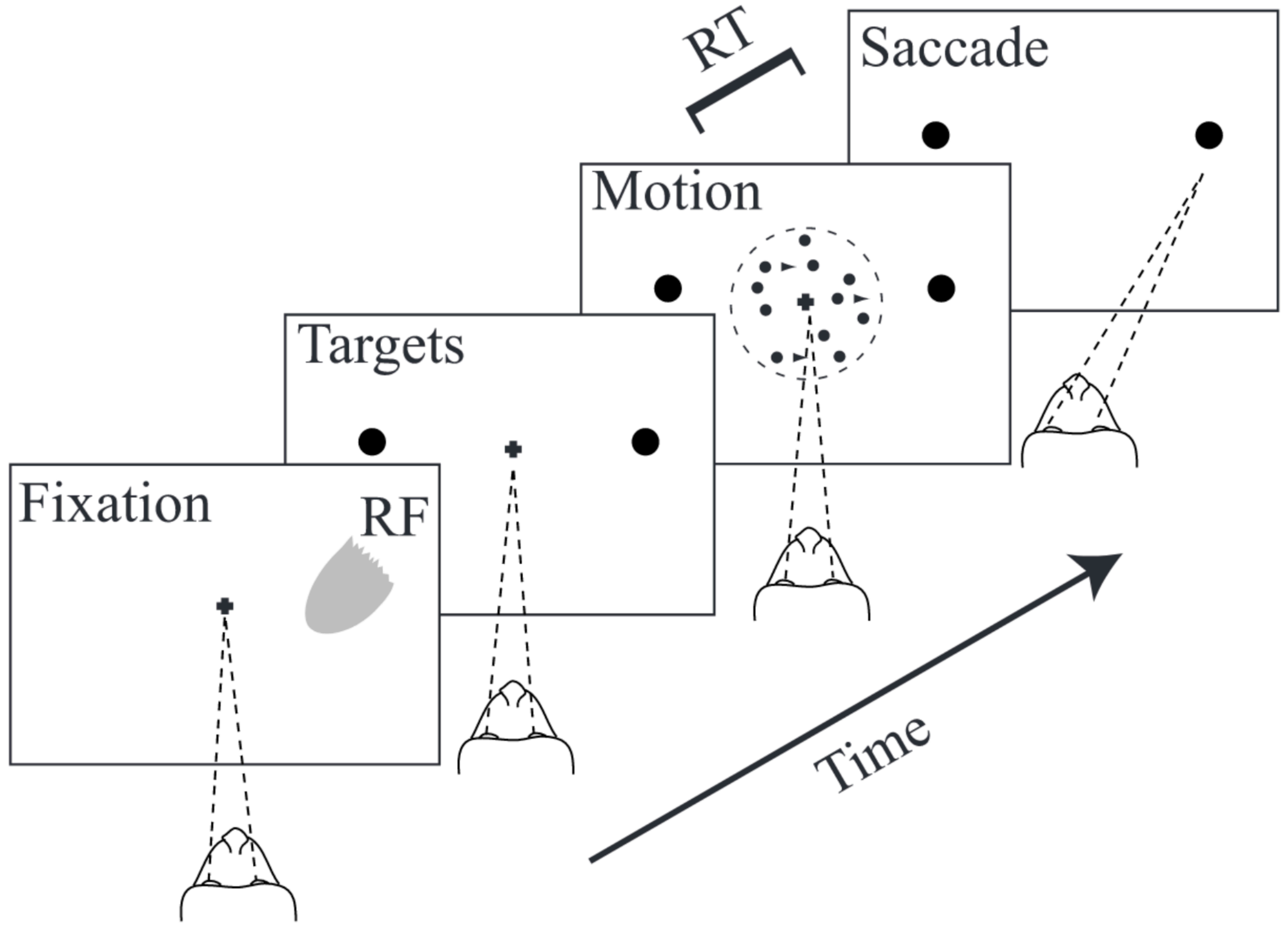
Studying decision-making in the brain

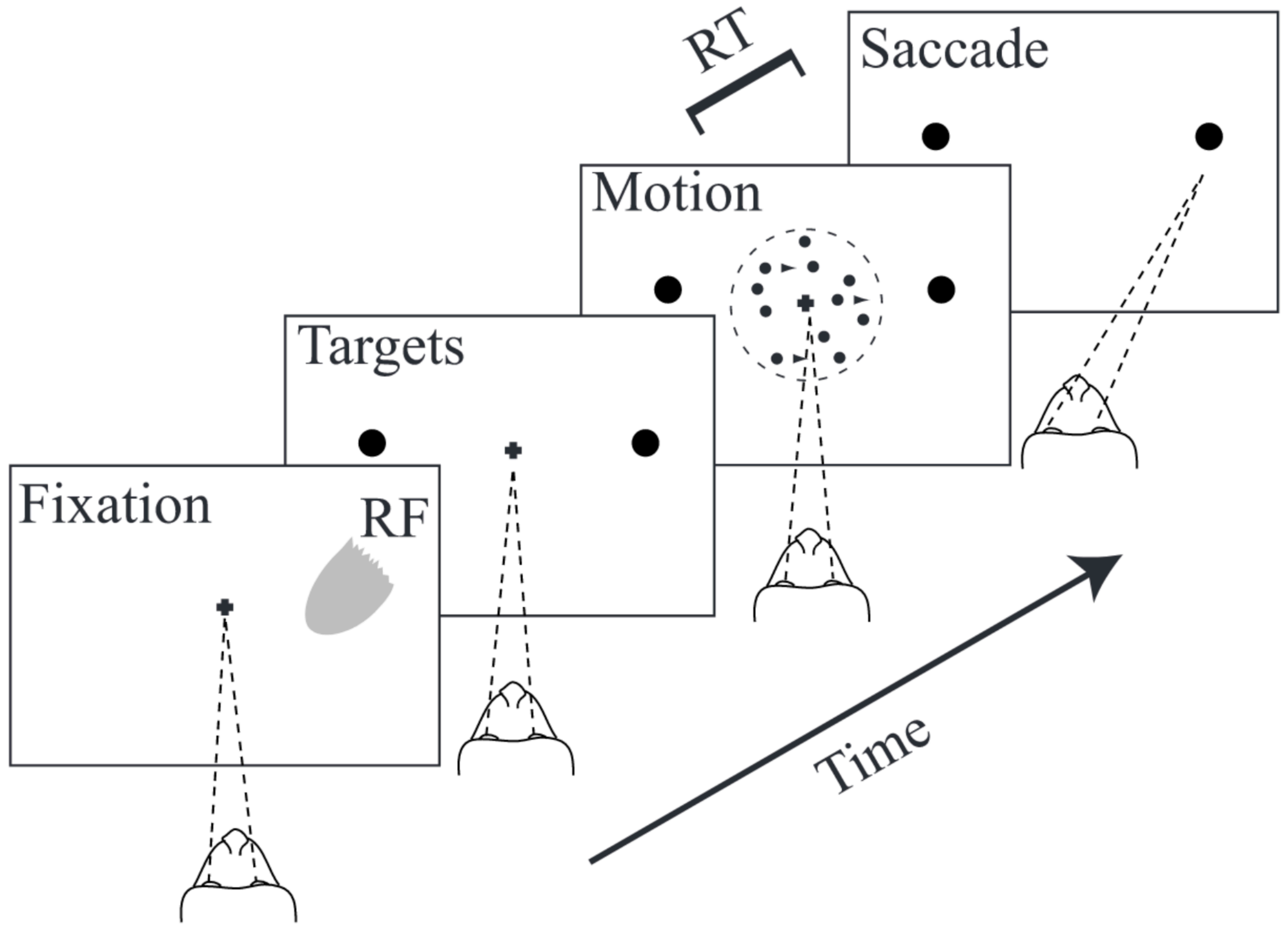
- Start simple: perceptual decision-making
- Random dot motion task
- Behavioral data:
  - reaction times and choices
  - $x = (r, c)$

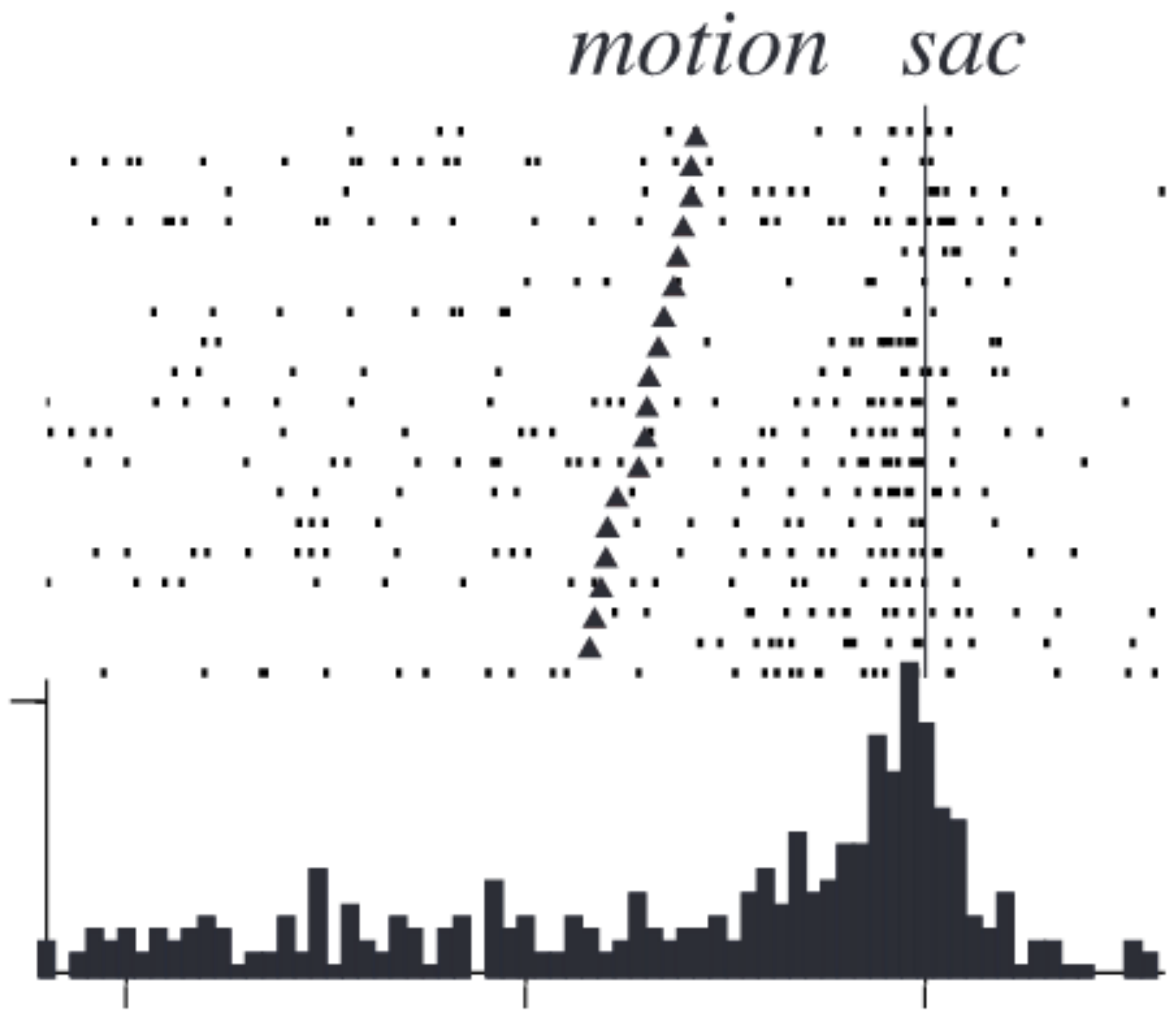


Newsome & Pare, 1988; Roitmann & Shadlen, 2002; Sanchez 2014

Studying decision-making in the brain

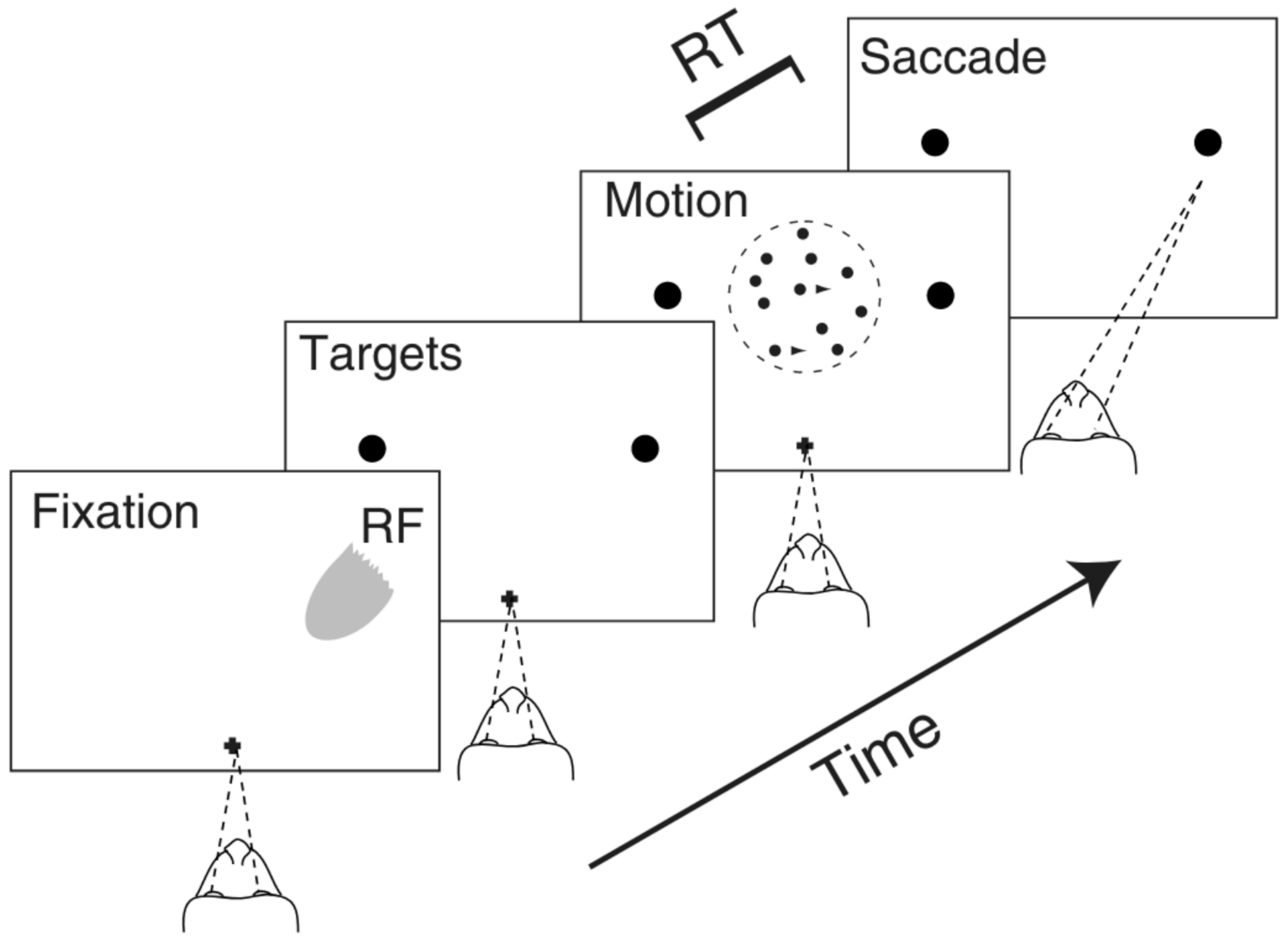
- Start simple: perceptual decision-making
- Random dot motion task
- Behavioral data:
  - reaction times and choices
  - $x = (r, c)$
- Neural data: recordings from single cells





Newsome & Pare, 1988; Roitmann & Shadlen, 2002; Sanchez 2014

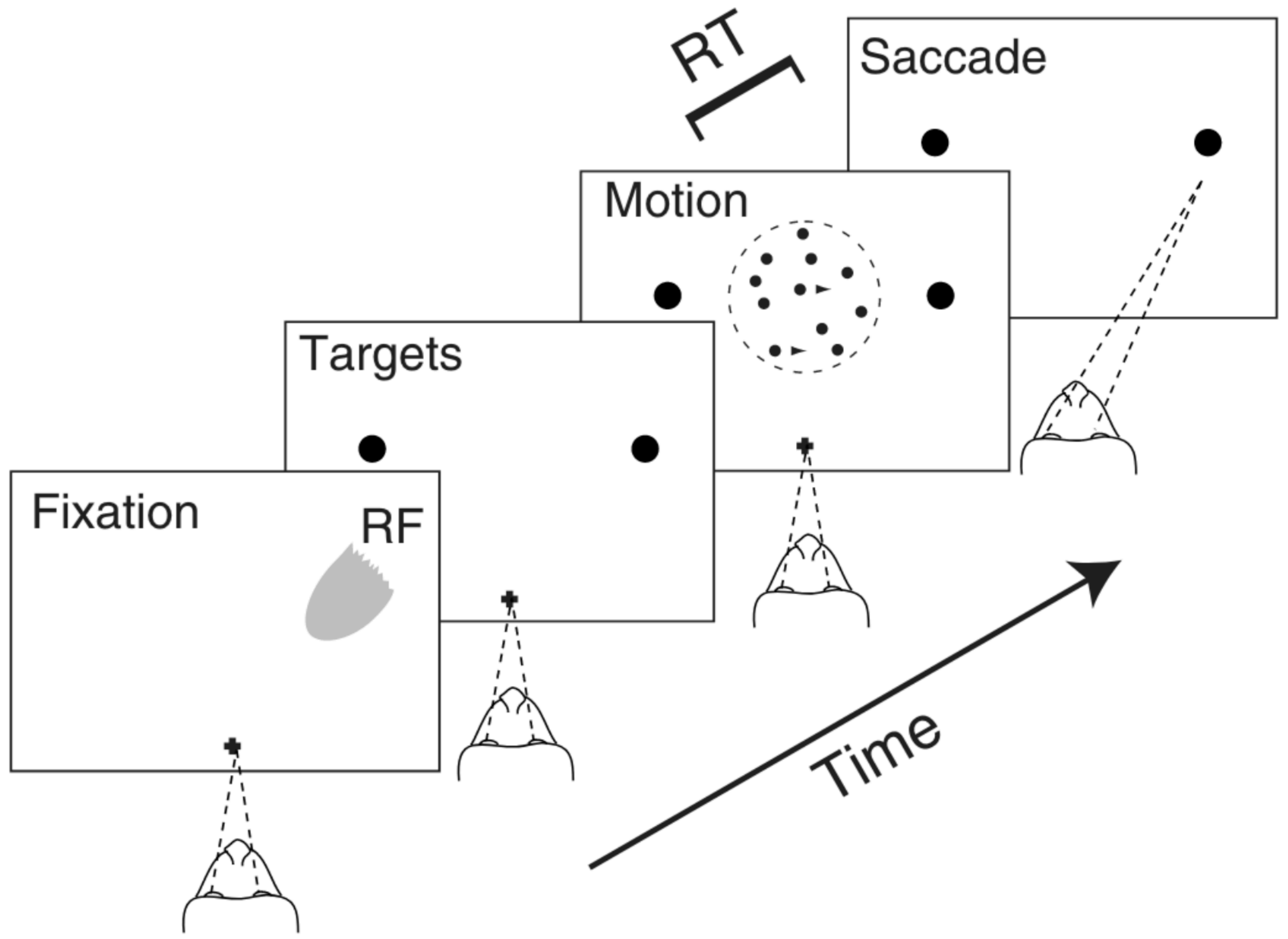
A computational model for decision-making



data:

Newsome & Pare, 1988; Roitmann & Shadlen, 2002

A computational model for decision-making



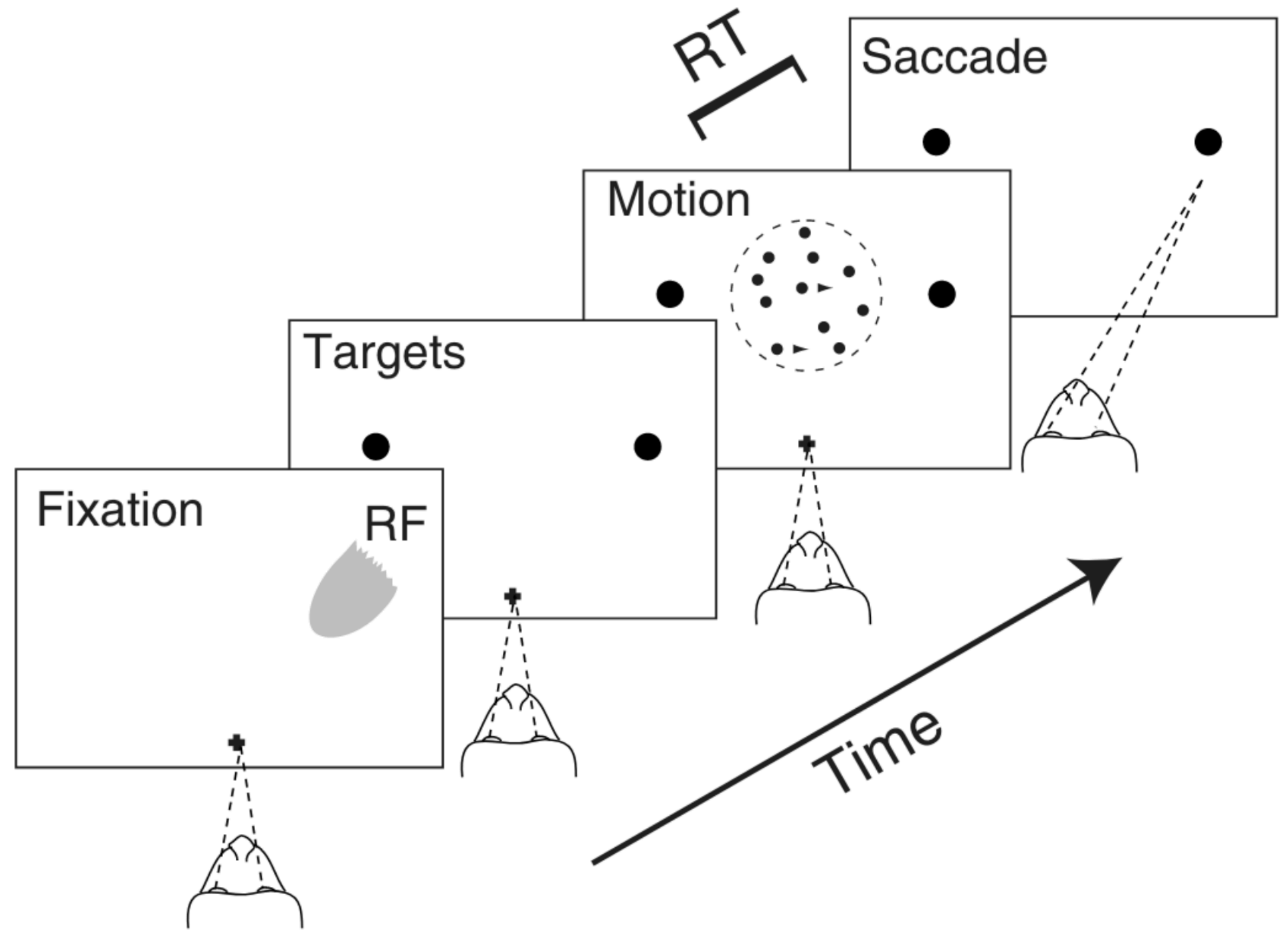
data:

- reaction times and choices (+neural data)

$$x = (r, c)$$

Newsome & Pare, 1988; Roitmann & Shadlen, 2002

A computational model for decision-making



data:

- reaction times and choices (+neural data)

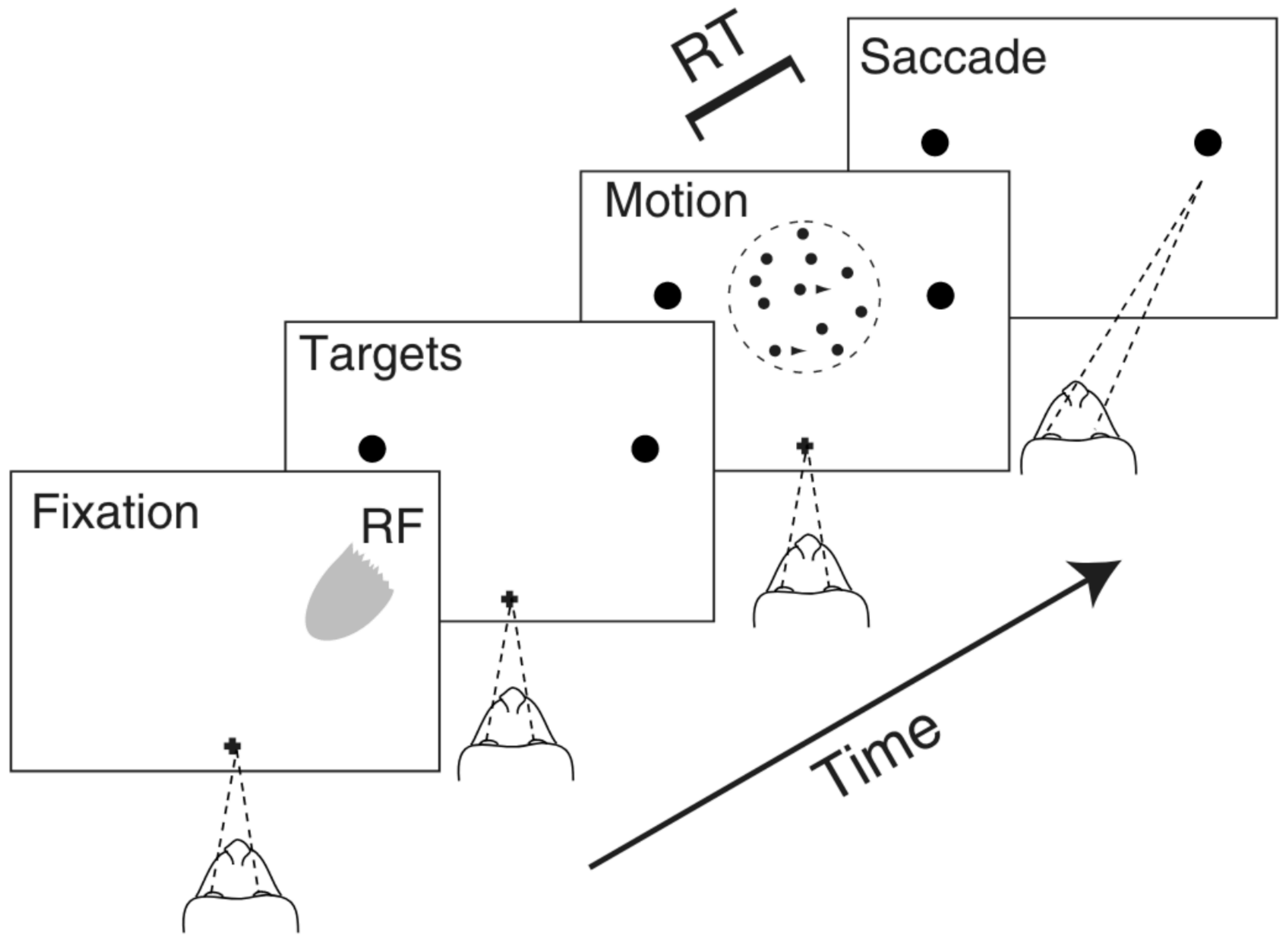
$$x = (r, c)$$

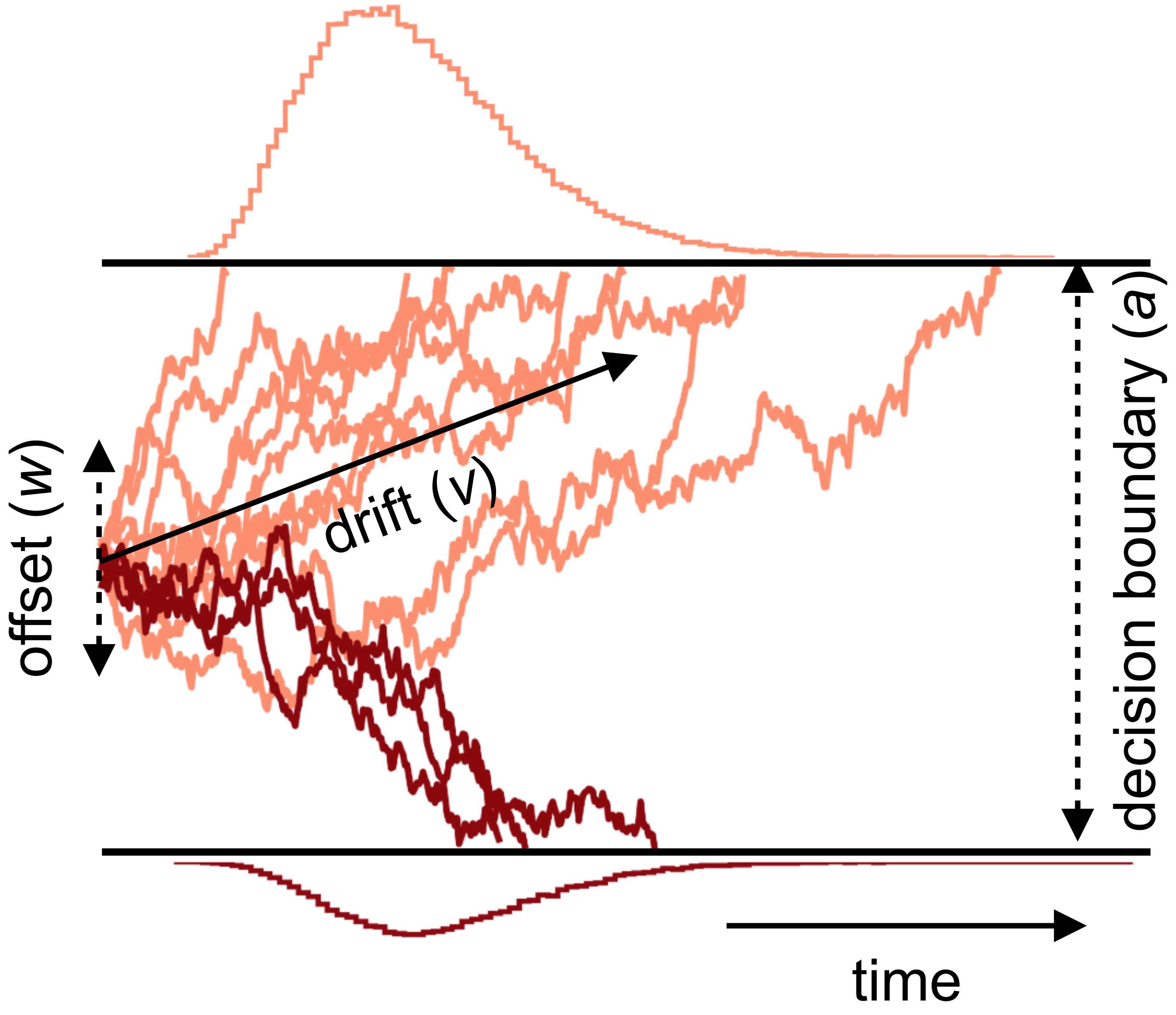
- many repetitions (trials)

$$X = \{r_j, c_j\}_{j=1}^{M}$$

Newsome & Pare, 1988; Roitmann & Shadlen, 2002

A computational model for decision-making





drift v (sensory evidence)

boundary a

offset w

non-decision time τ

data:

- reaction times and choices (+neural data)

$$x = (r, c)$$

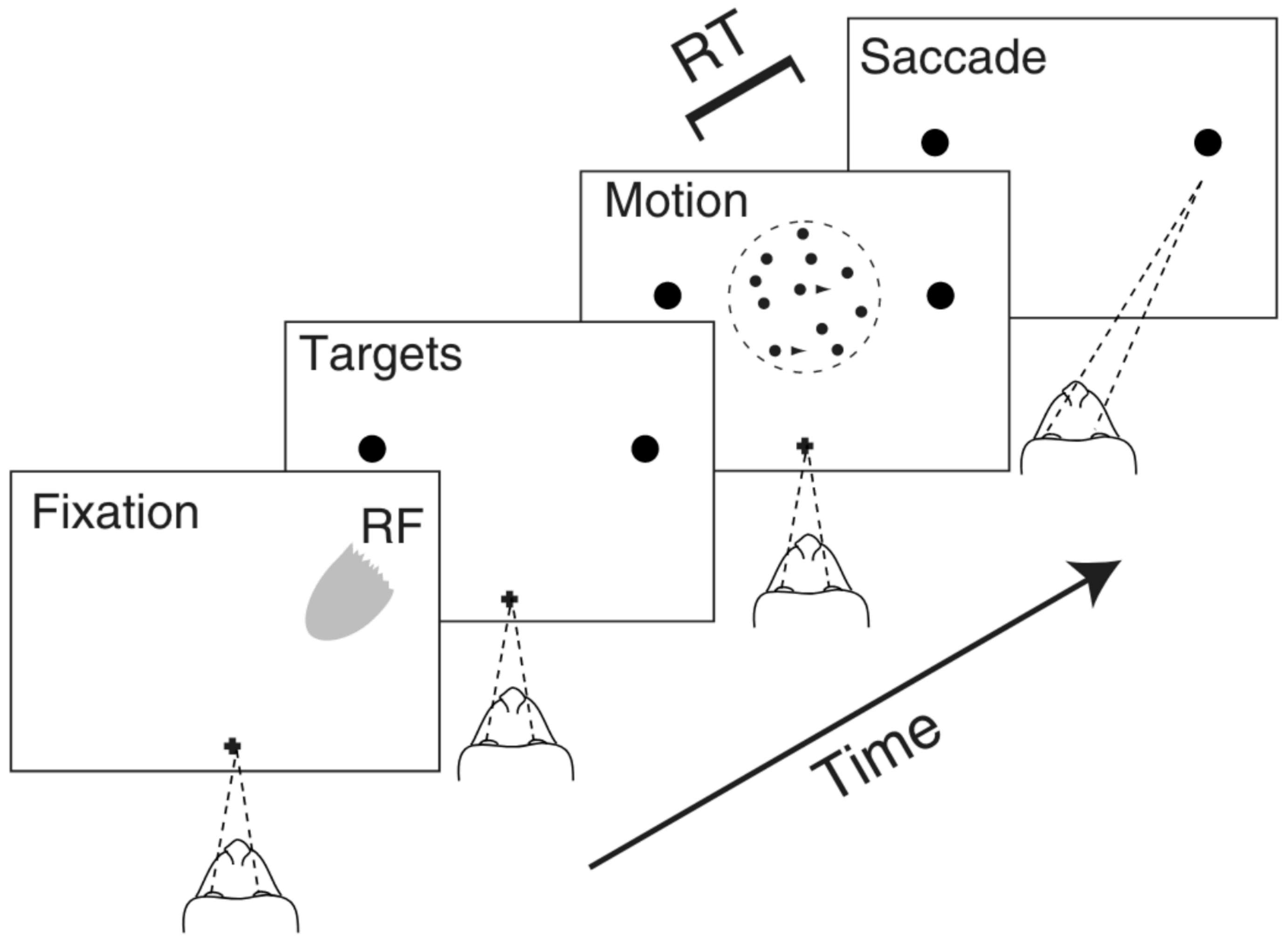
- many repetitions (trials)

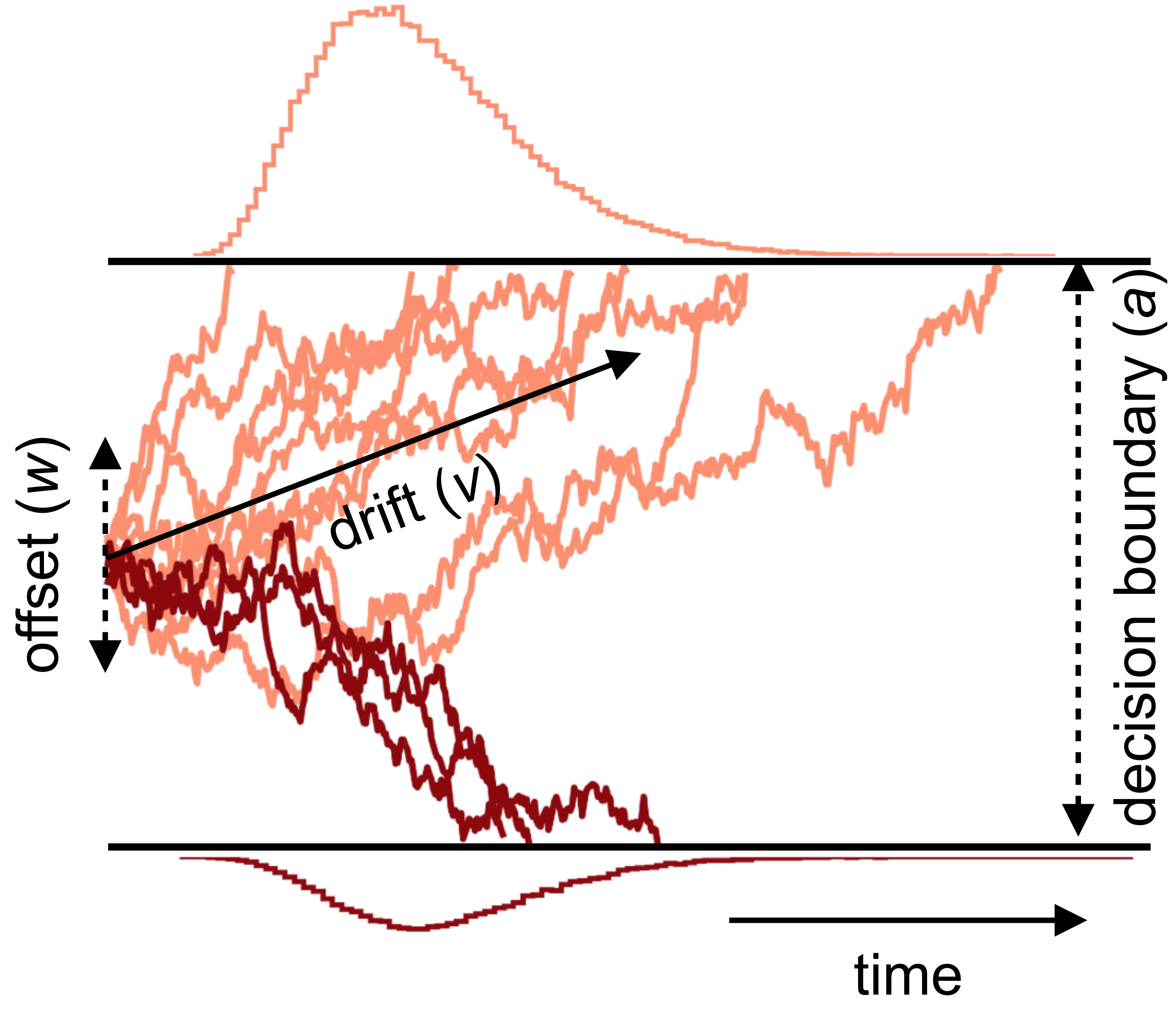
$$X = \{r_j, c_j\}_{j=1}^{M}$$

model: Drift-Diffusion Model (DDM)

Newsome & Pare, 1988; Roitmann & Shadlen, 2002

A computational model for decision-making





drift v (sensory evidence)

boundary a

offset w

non-decision time τ

data:

- reaction times and choices (+neural data)

$$x = (r, c)$$

- many repetitions (trials)

$$X = \{r_j, c_j\}_{j=1}^{M}$$

model: Drift-Diffusion Model (DDM)

$$dY = v\,dt + \sigma\,dW$$

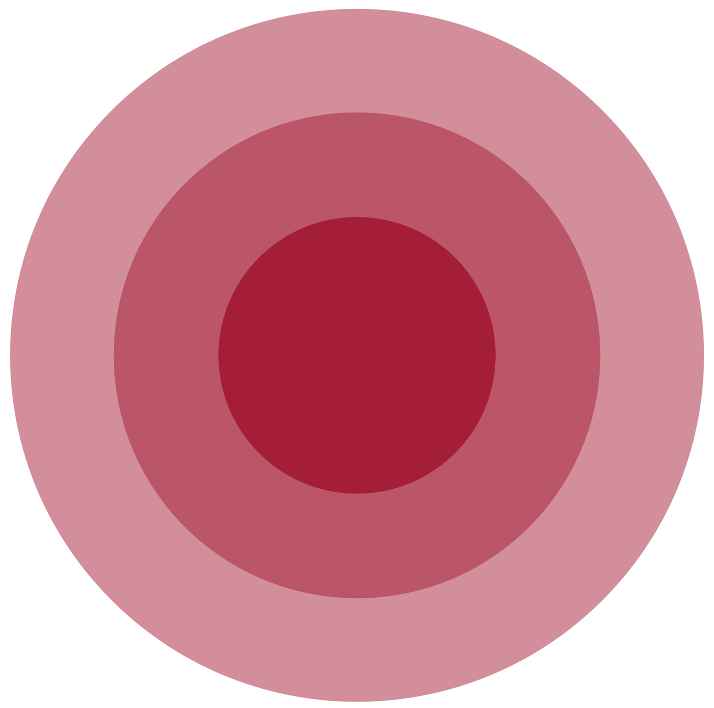
$$\theta = [v, a, w, \tau]$$

Newsome & Pare, 1988; Roitmann & Shadlen, 2002

Bayesian inference for the drift-diffusion model

forward model

parameters θ

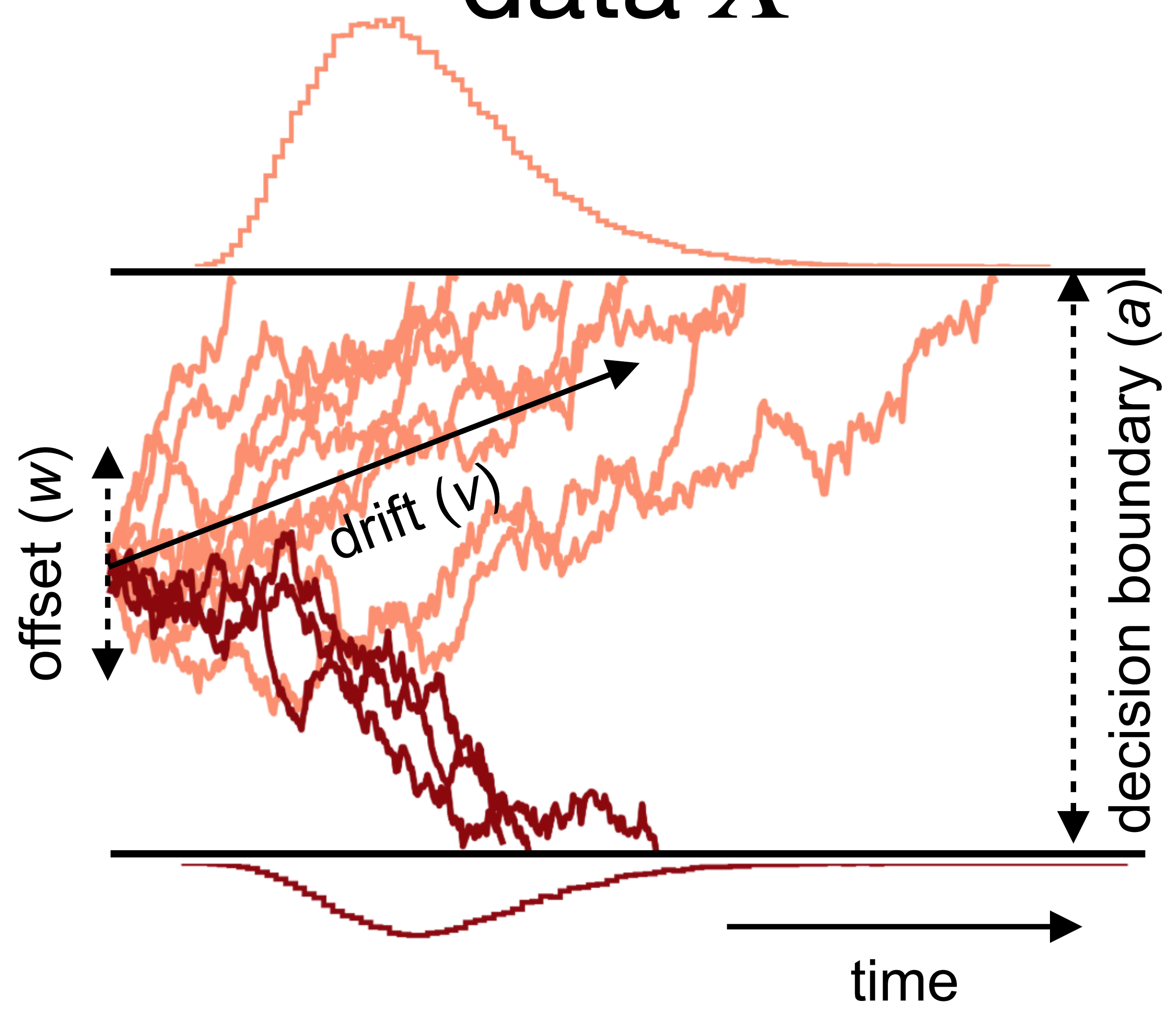


$\theta \sim p(\theta)$

$$X_o = \{r_j, c_j\}_{j=1}^{M}$$

$$p(\theta \,|\, X_o) \propto p(X_o \,|\, \theta)\, p(\theta)$$

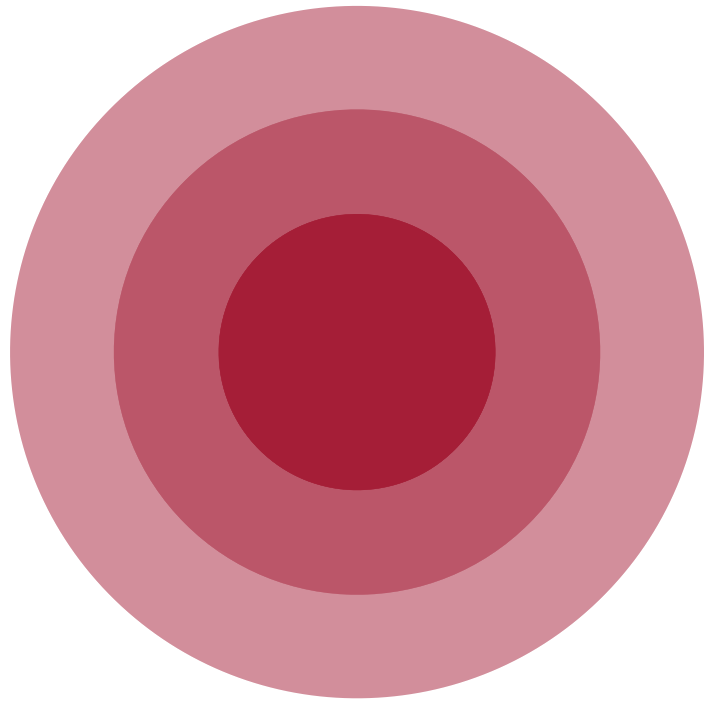
data X



Bayesian inference for the drift-diffusion model

forward model

parameters θ

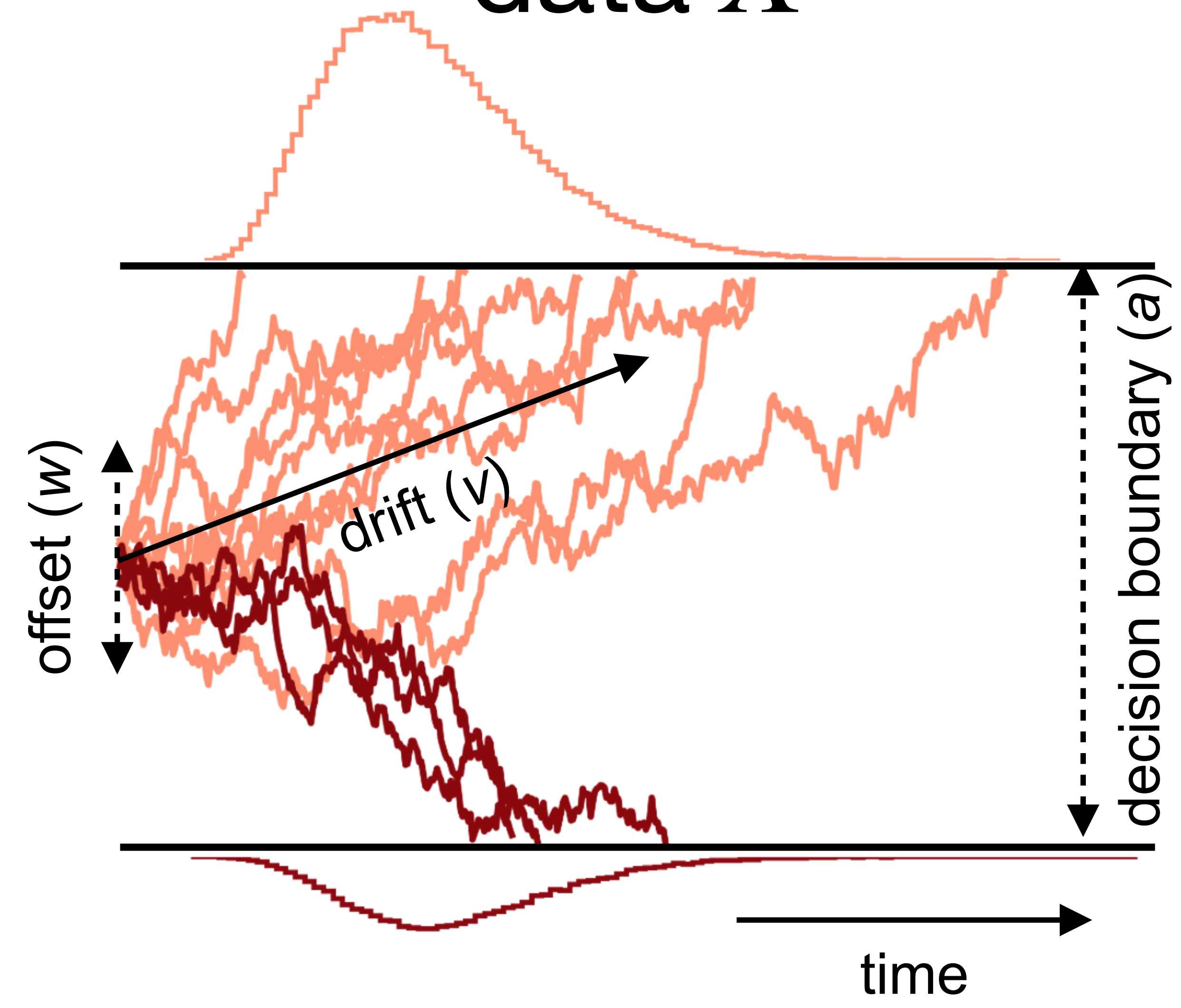


$\theta \sim p(\theta)$

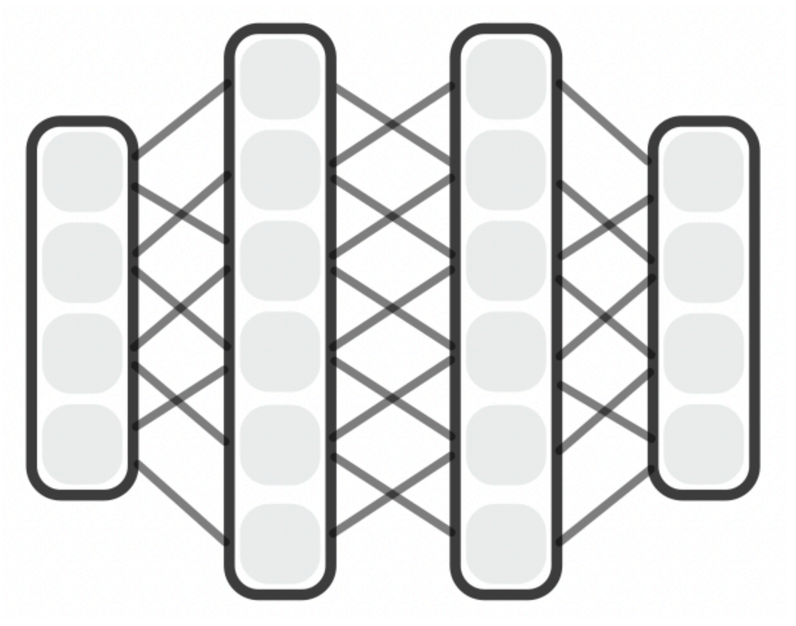
$$X_o = \{r_j, c_j\}_{j=1}^{M}$$

$$p(\theta \mid X_o) \propto p(X_o \mid \theta)\, p(\theta)$$

data X



simulation-based inference



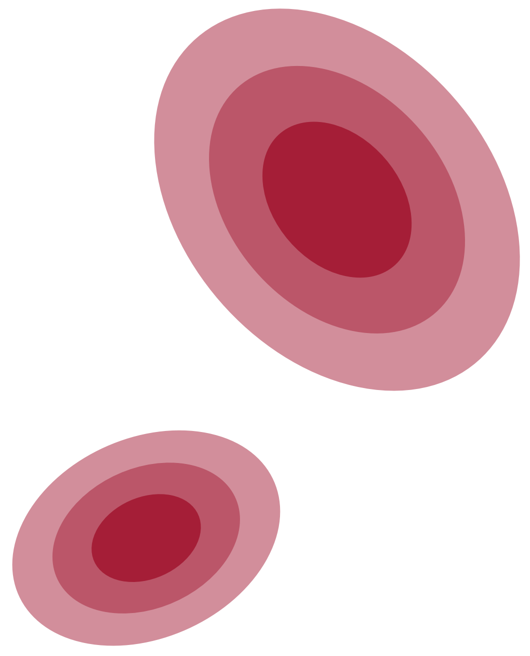
training data

$\{(\theta_1, X_1), (\theta_2, X_2), \ldots\}$

Bayesian inference for the drift-diffusion model

forward model

parameters θ

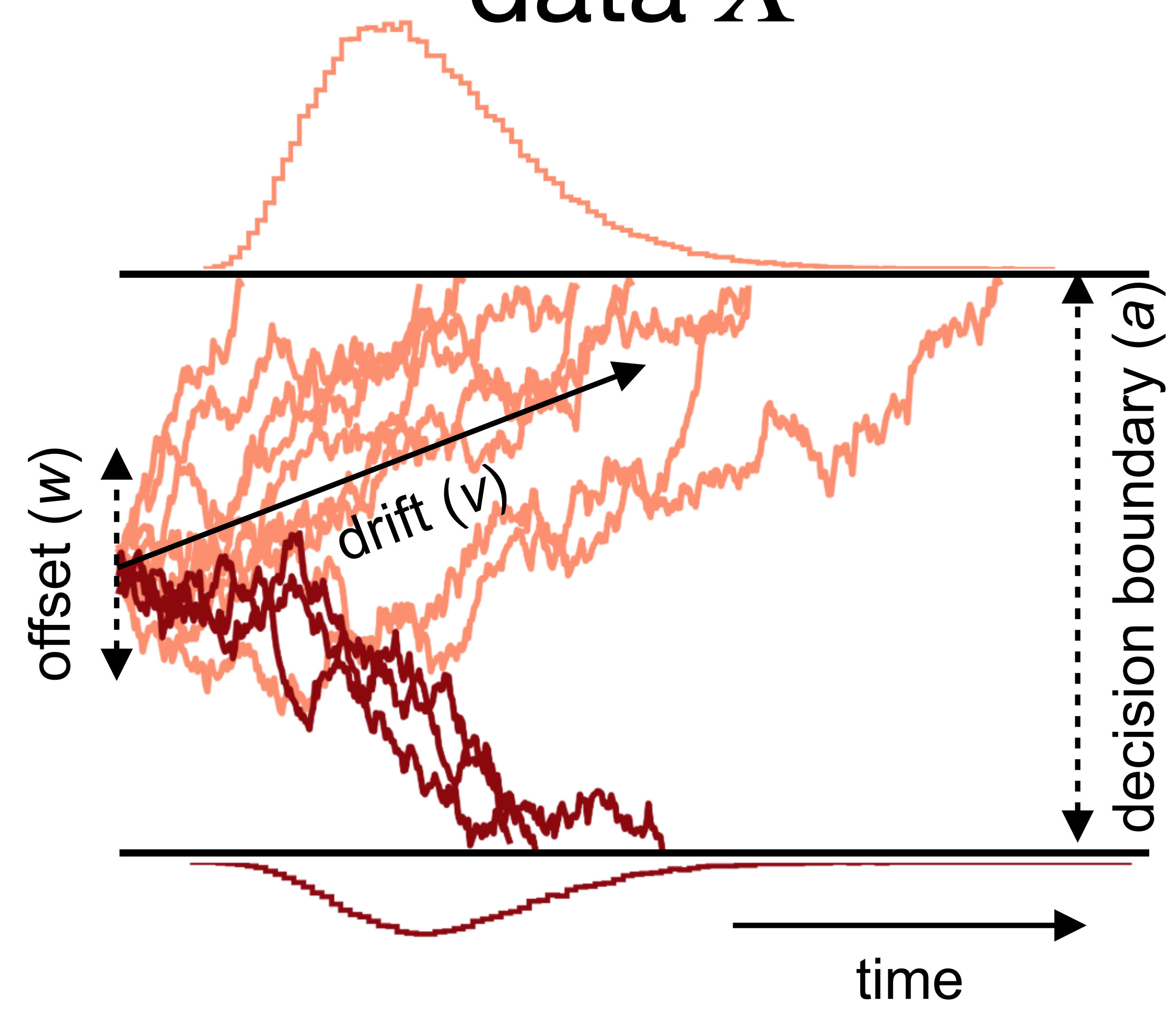


$p(\theta | x)$

$$X_o = \{r_j, c_j\}_{j=1}^{M}$$

$$p(\theta | X_o) \propto p(X_o | \theta)\, p(\theta)$$

data X



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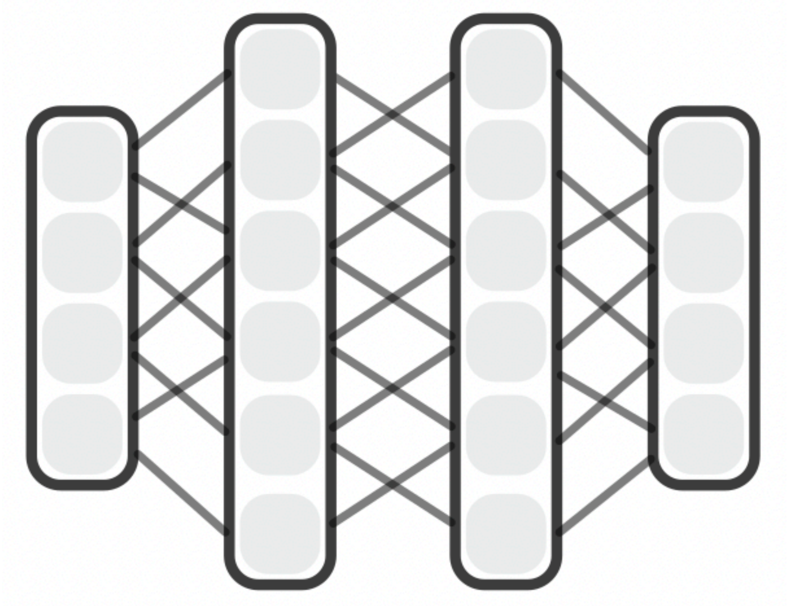


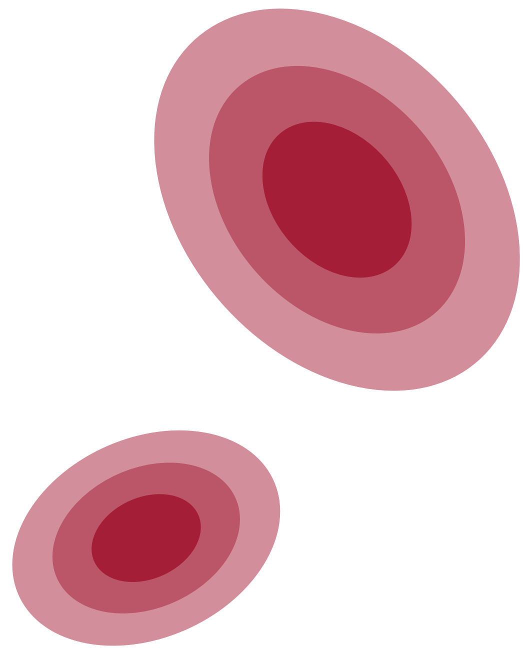
training data

$\{(\theta_1, X_1), (\theta_2, X_2), \dots\}$

Bayesian inference for the drift-diffusion model

forward model

parameters θ

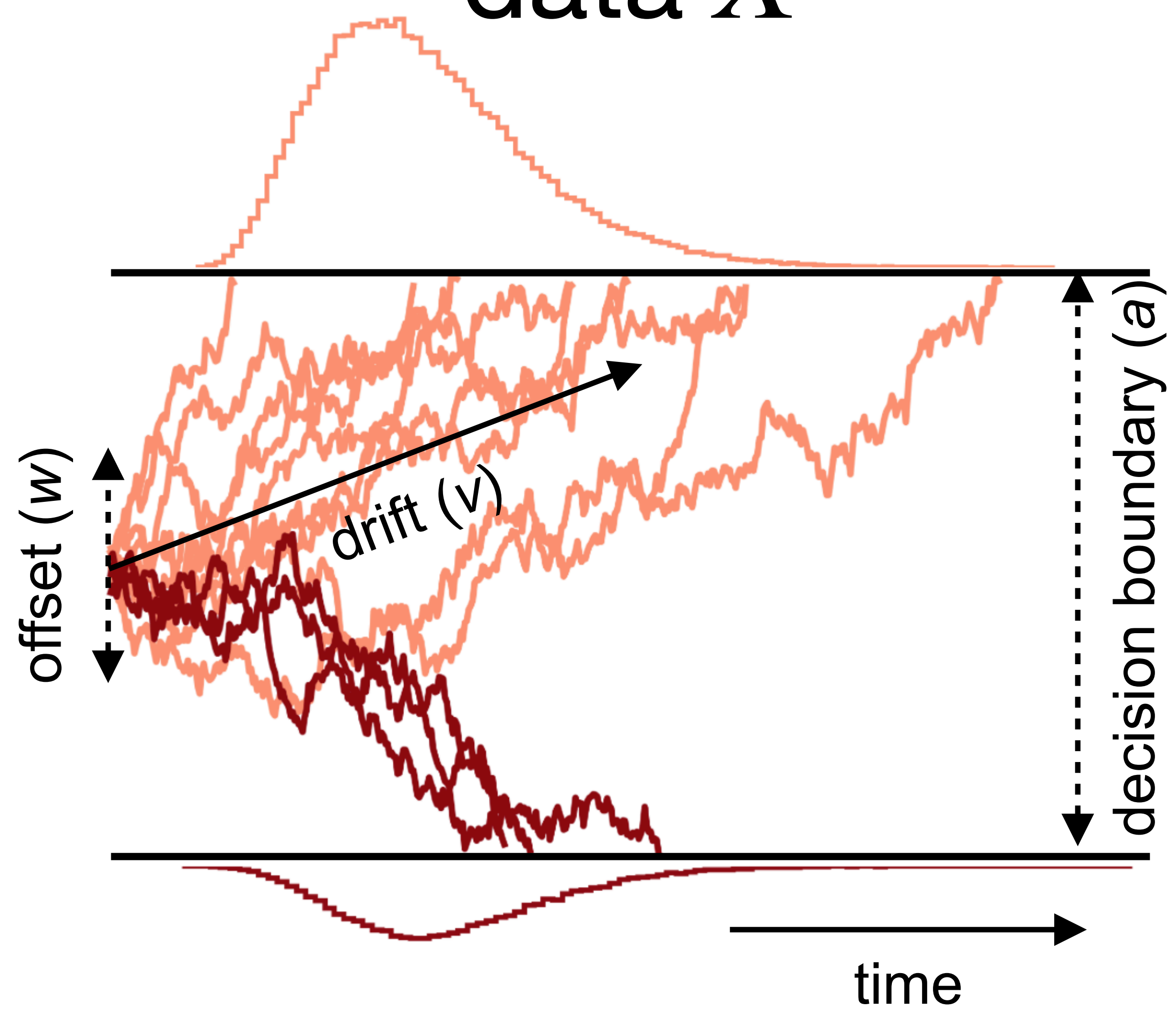


$p(\theta | x)$

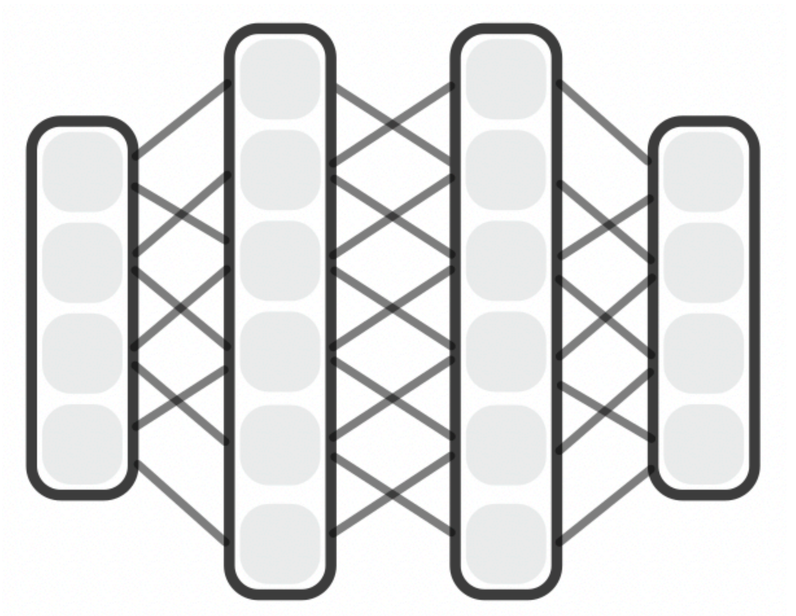
$$X_o = \{r_j, c_j\}_{j=1}^{M}$$

$$p(\theta | X_o) \propto \boxed{p(X_o | \theta)} p(\theta)$$

data X



simulation-based inference



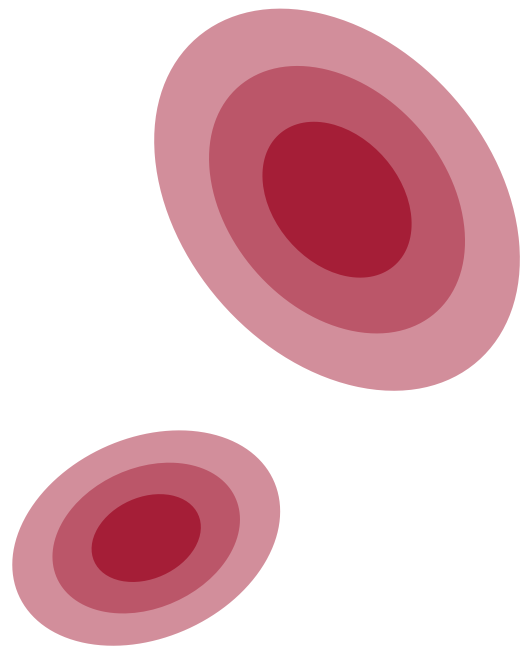
training data

$\{(\theta_1, X_1), (\theta_2, X_2), \ldots\}$

Bayesian inference for the drift-diffusion model

forward model

parameters θ



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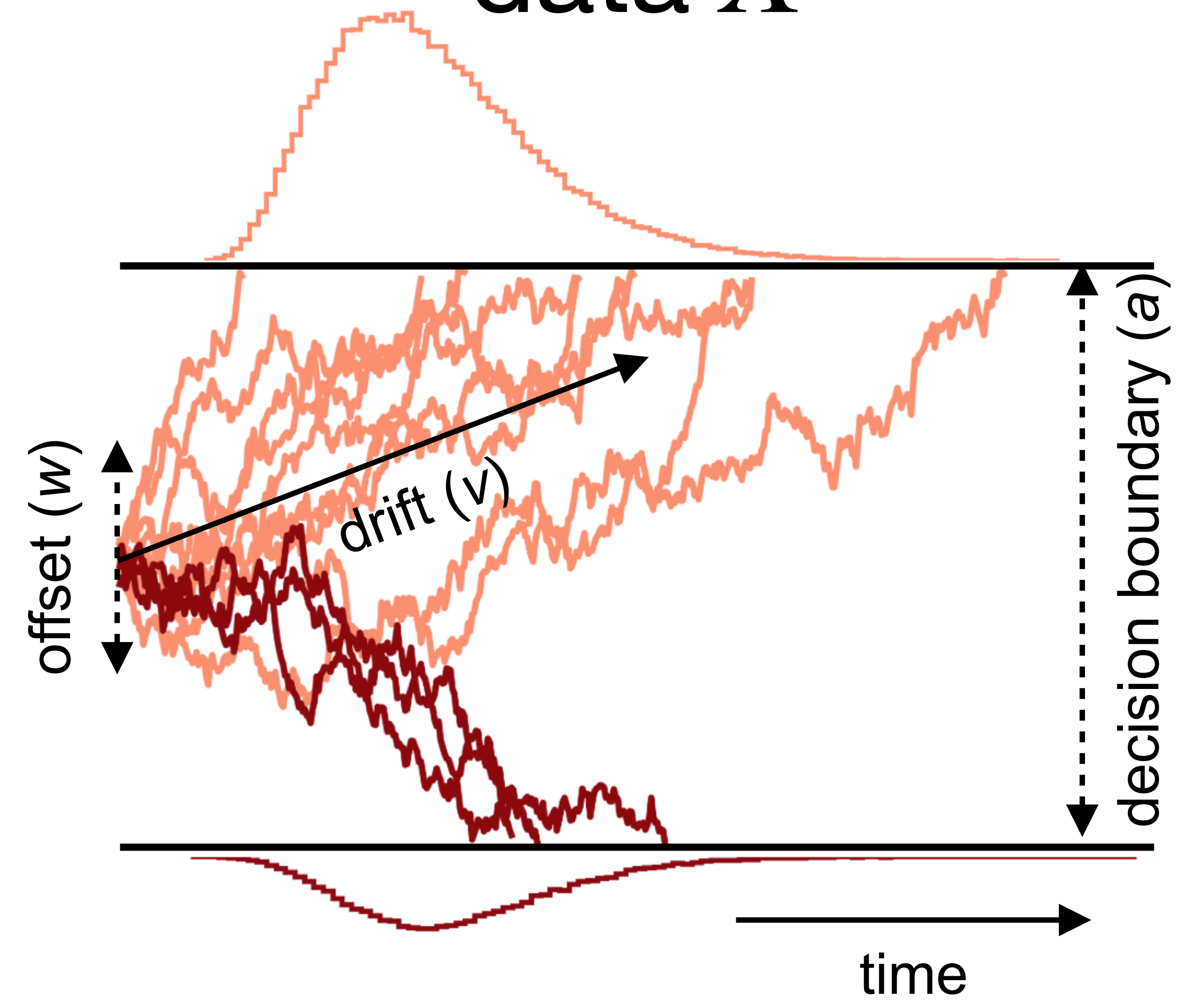
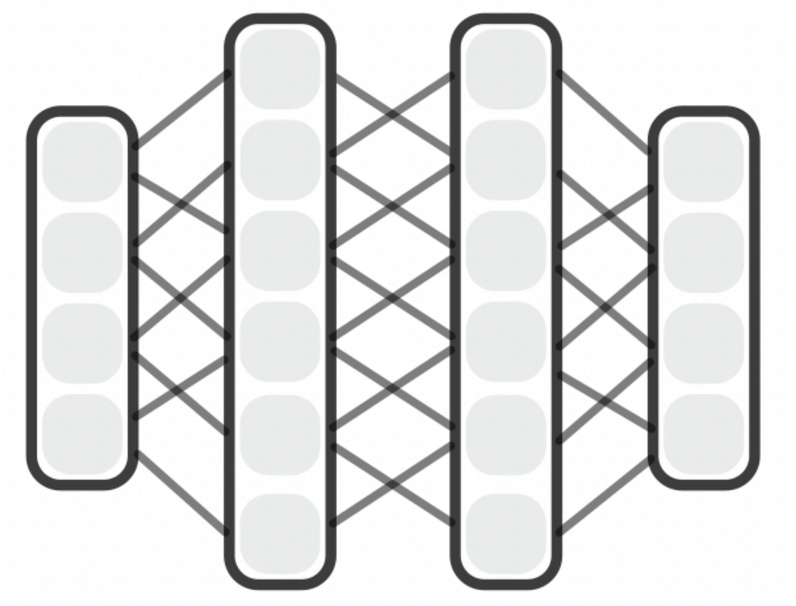
$$p(\theta | X_o) \propto p(X_o | \theta) p(\theta)$$

data X



simulation-based inference



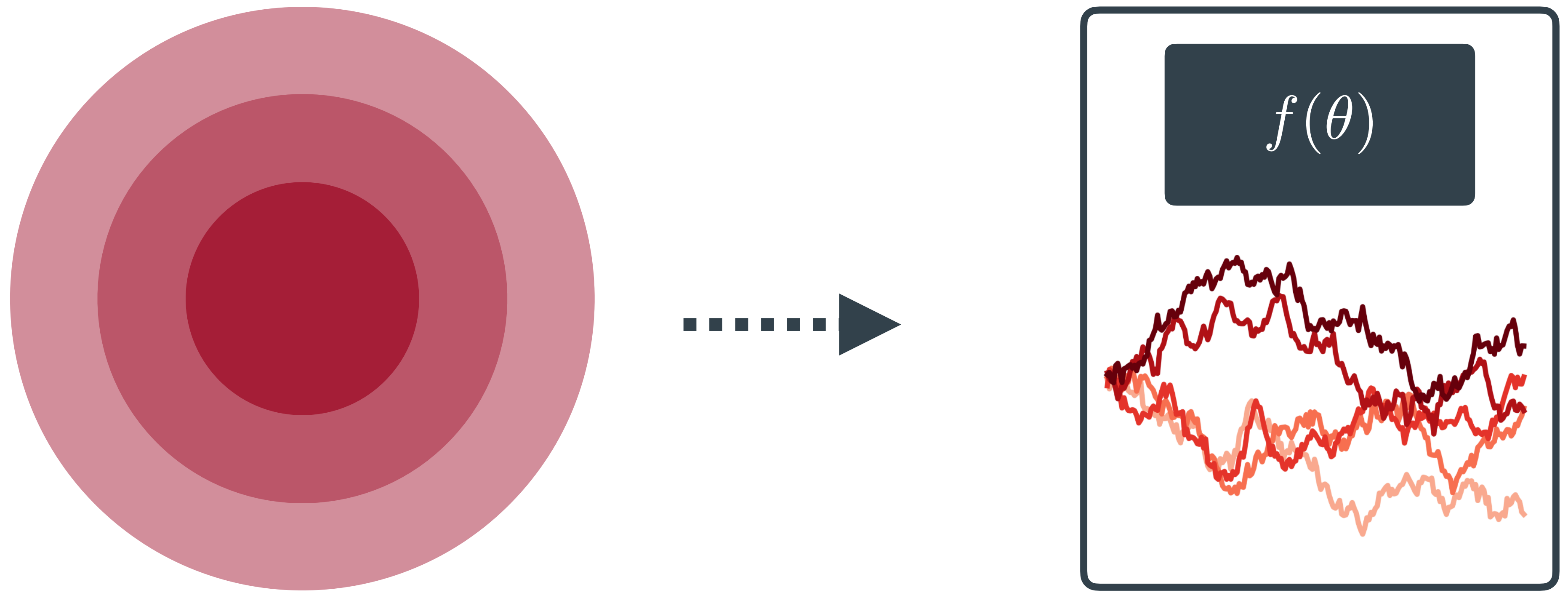
training data

$\{(\theta_1, X_1), (\theta_2, X_2), \ldots\}$

Neural Likelihood Estimation (NLE)

prior

simulated data



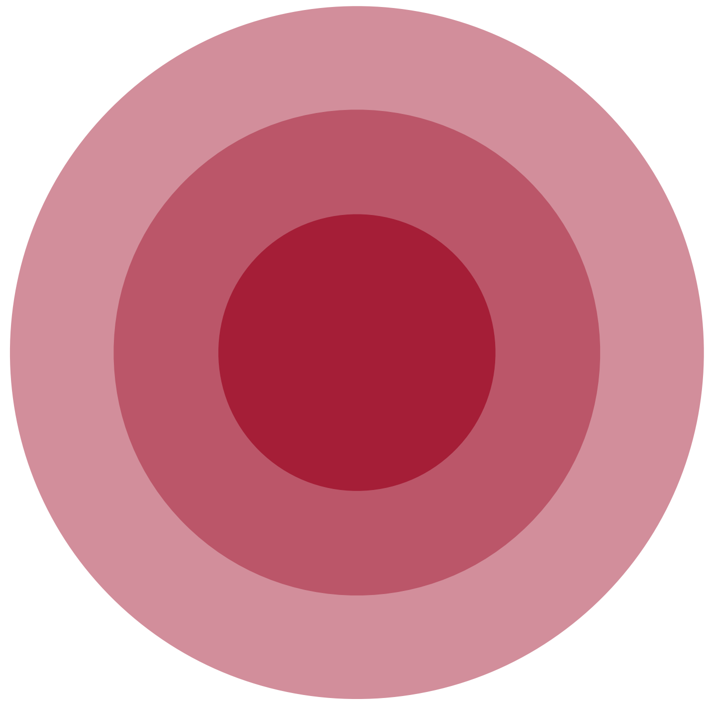
$\theta_i \sim p(\theta)$

$\{\theta_i, x_i\}_{i=1}^{N}$

Wood, 2010; Blum et al. 2010; Papamakarios et al. 2016, 2018

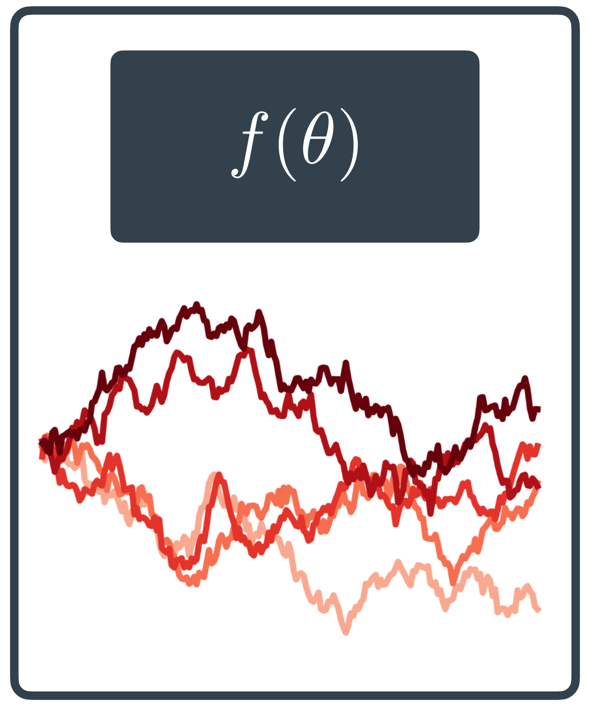
Neural Likelihood Estimation (NLE)

prior



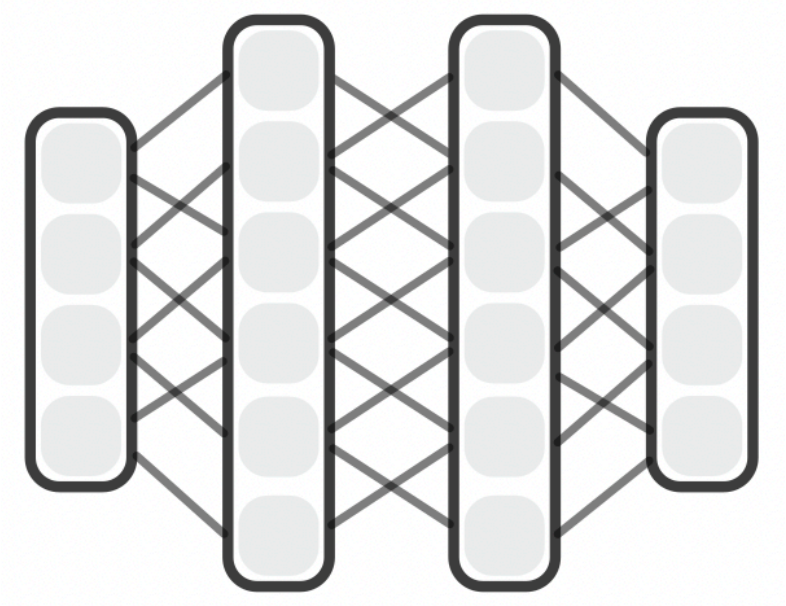
$\theta_i \sim p(\theta)$

simulated data



$\{\theta_i, x_i\}_{i=1}^{N}$

density estimator



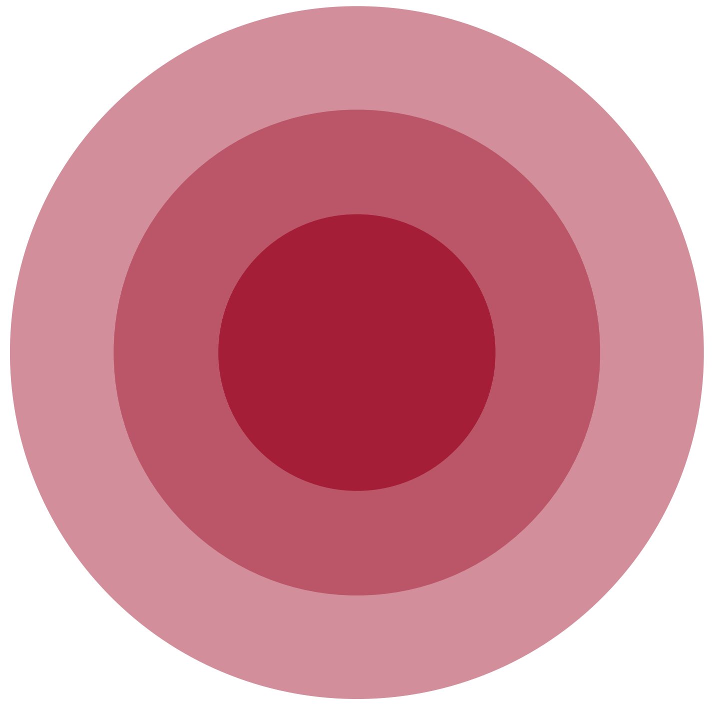
$\underset{\phi}{\operatorname{argmin}}\ \mathcal{L}(\phi)$

- train an artificial neural network (NN) to approximate the **likelihood**

Wood, 2010; Blum et al. 2010; Papamakarios et al. 2016, 2018

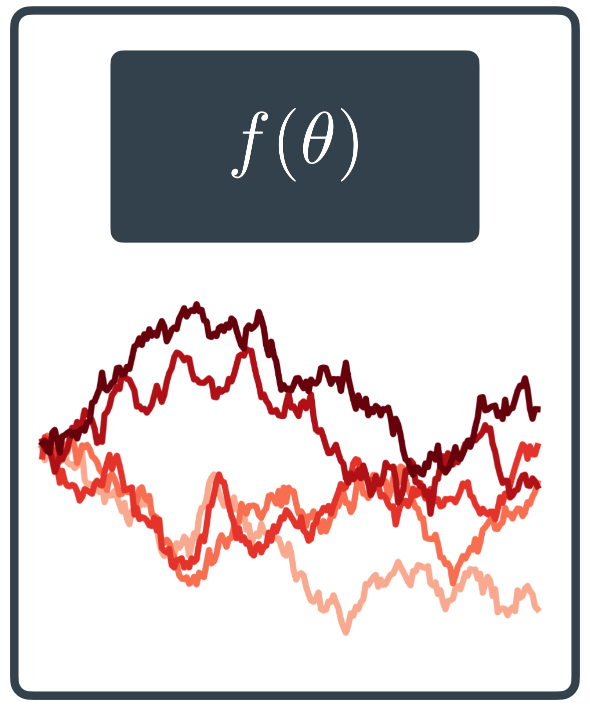
Neural Likelihood Estimation (NLE)

prior



$\theta_i \sim p(\theta)$

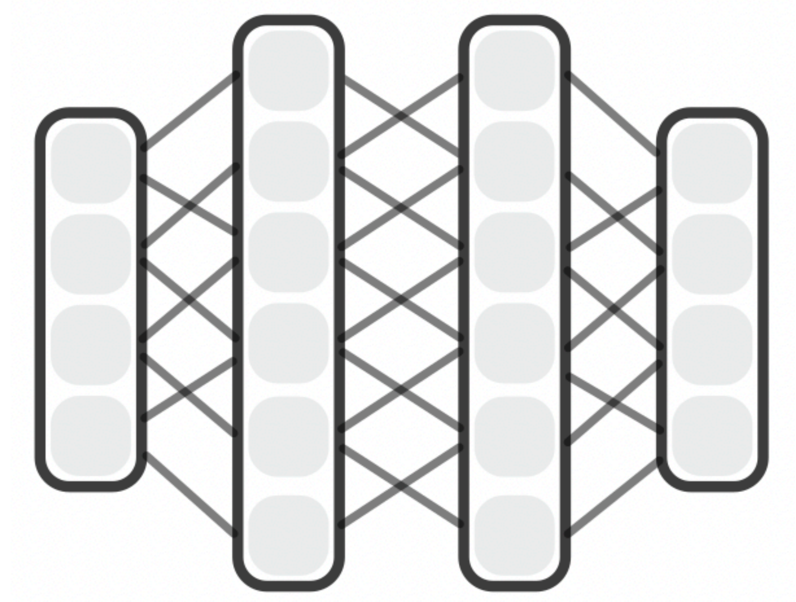
simulated data



$\{\theta_i, x_i\}_{i=1}^N$

density estimator

$\theta_i \rightarrow$



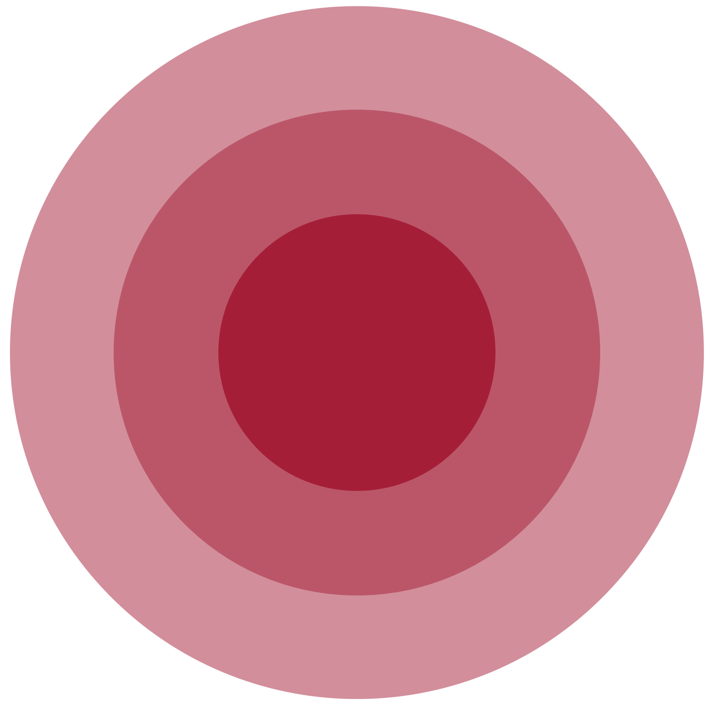
$\underset{\phi}{\text{argmin}}\ \mathcal{L}(\phi)$

- train an artificial neural network (NN) to approximate the **likelihood**

Wood, 2010; Blum et al. 2010; Papamakarios et al. 2016, 2018

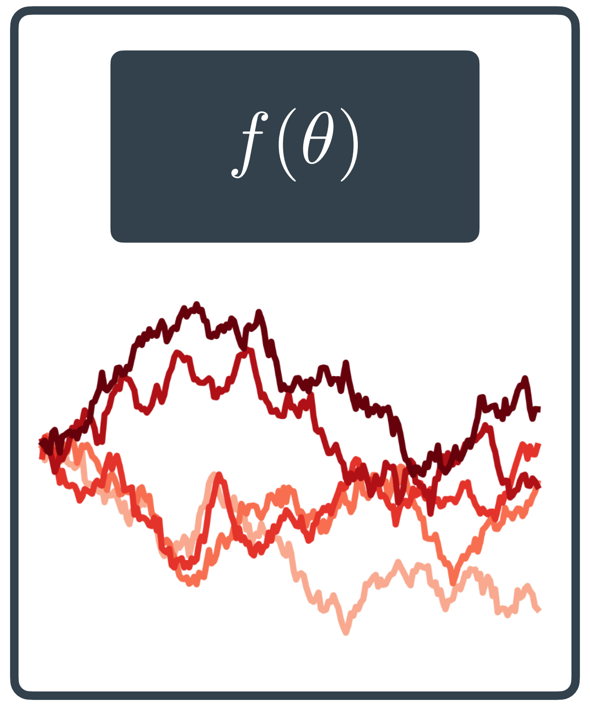
Neural Likelihood Estimation (NLE)

prior



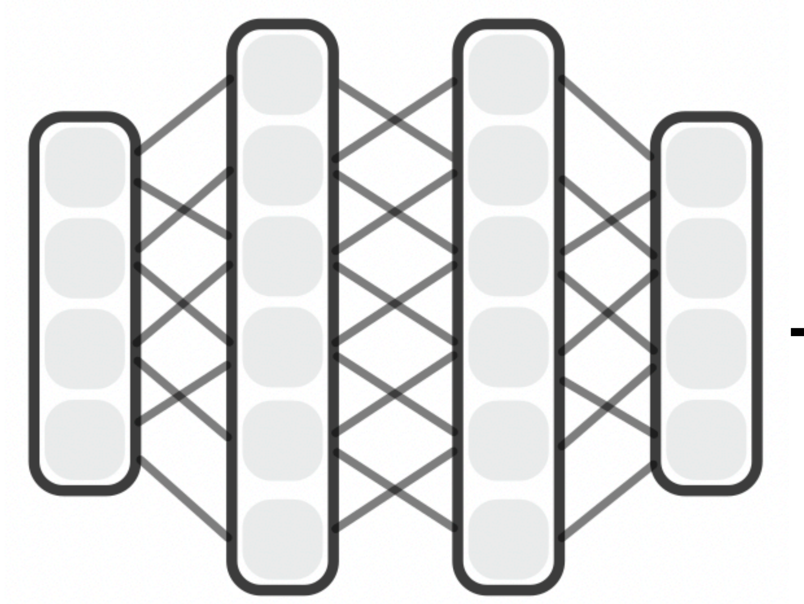
$\theta_i \sim p(\theta)$

simulated data



$\{\theta_i, x_i\}_{i=1}^N$

density estimator

$\theta_i \rightarrow$  $\rightarrow q_\phi(x \mid \theta_i)$

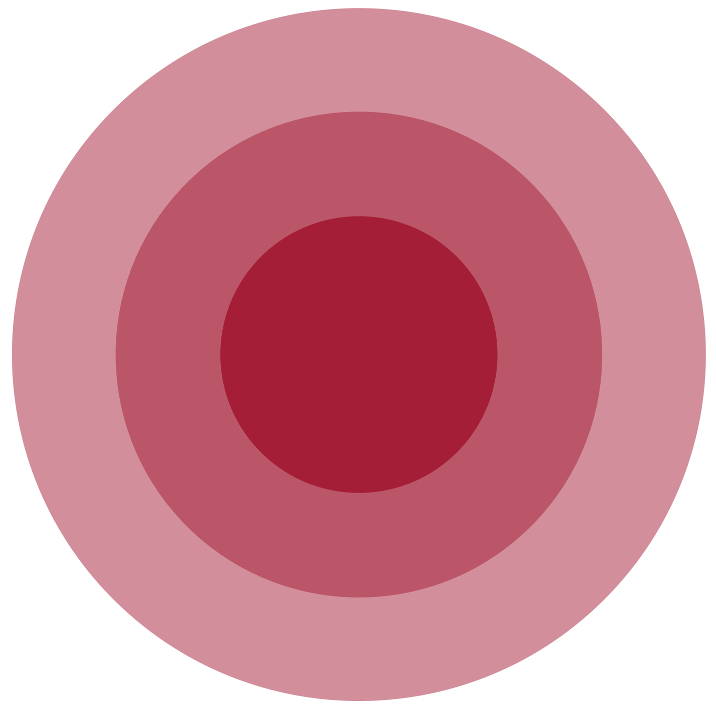
$$\underset{\phi}{\text{argmin}}\ \mathcal{L}(\phi)$$

- train an artificial neural network (NN) to approximate the **likelihood**

Wood, 2010; Blum et al. 2010; Papamakarios et al. 2016, 2018

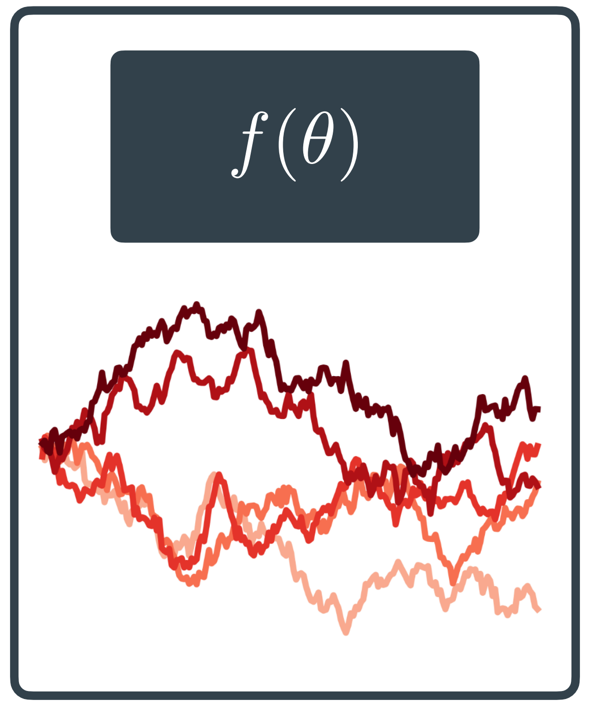
Neural Likelihood Estimation (NLE)

prior



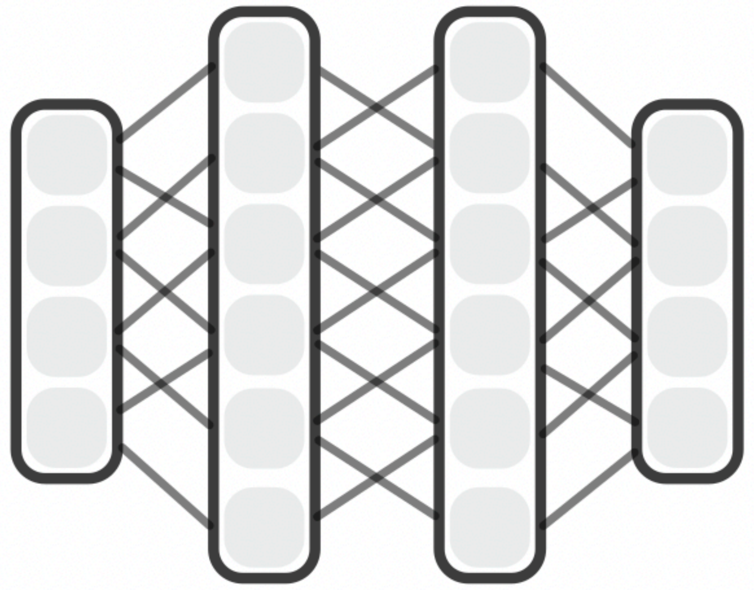
$\theta_i \sim p(\theta)$

simulated data



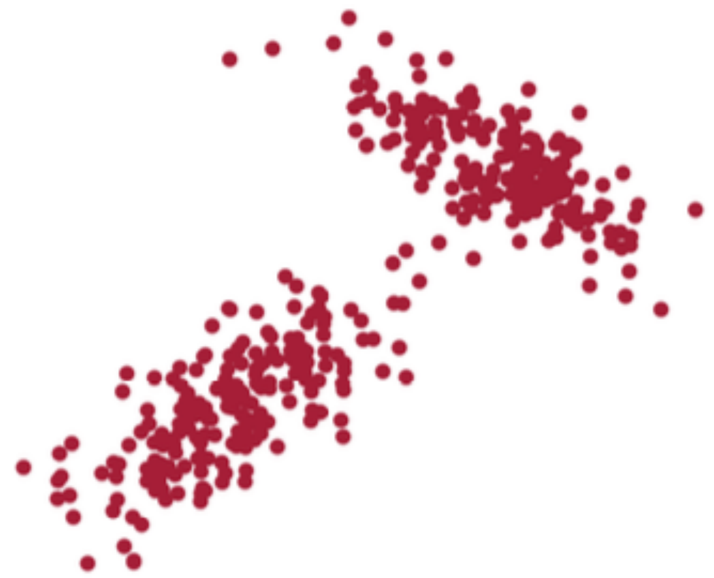
$\{\theta_i, x_i\}_{i=1}^{N}$

density estimator

$\theta_i \rightarrow$  $\rightarrow q_\phi(x \,|\, \theta_i)$

$$\underset{\phi}{\text{argmin}}\ \mathcal{L}(\phi)$$

posterior



$$p(\theta \,|\, x_o) \propto q(x_o \,|\, \theta)\, p(\theta)$$

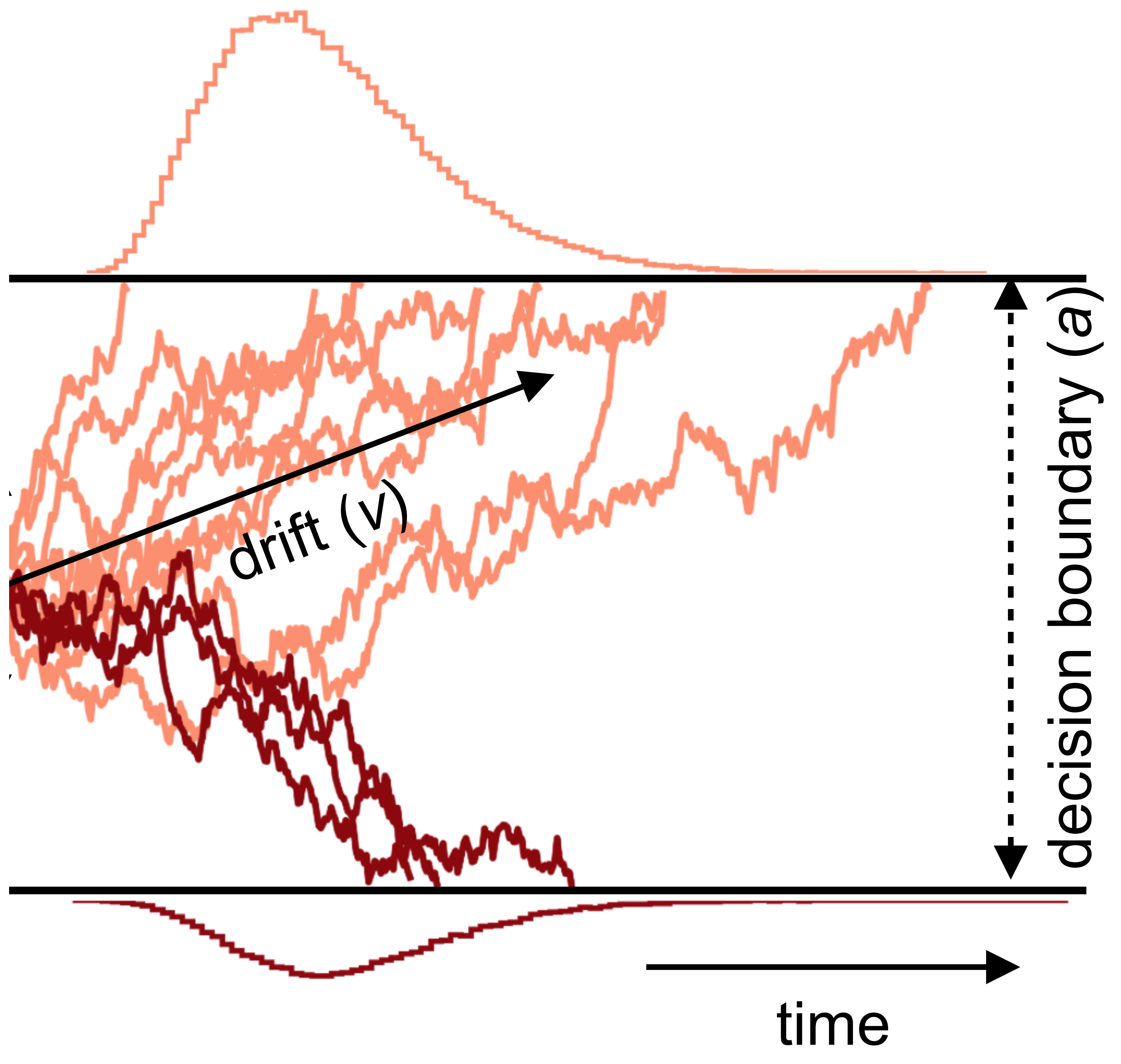
$$\theta \sim \hat{p}(\theta \,|\, x_o)$$

- train an artificial neural network (NN) to approximate the **likelihood**
- use Markov Chain Monte Carlo (**MCMC**) to obtain **posterior samples**

Wood, 2010; Blum et al. 2010; Papamakarios et al. 2016, 2018

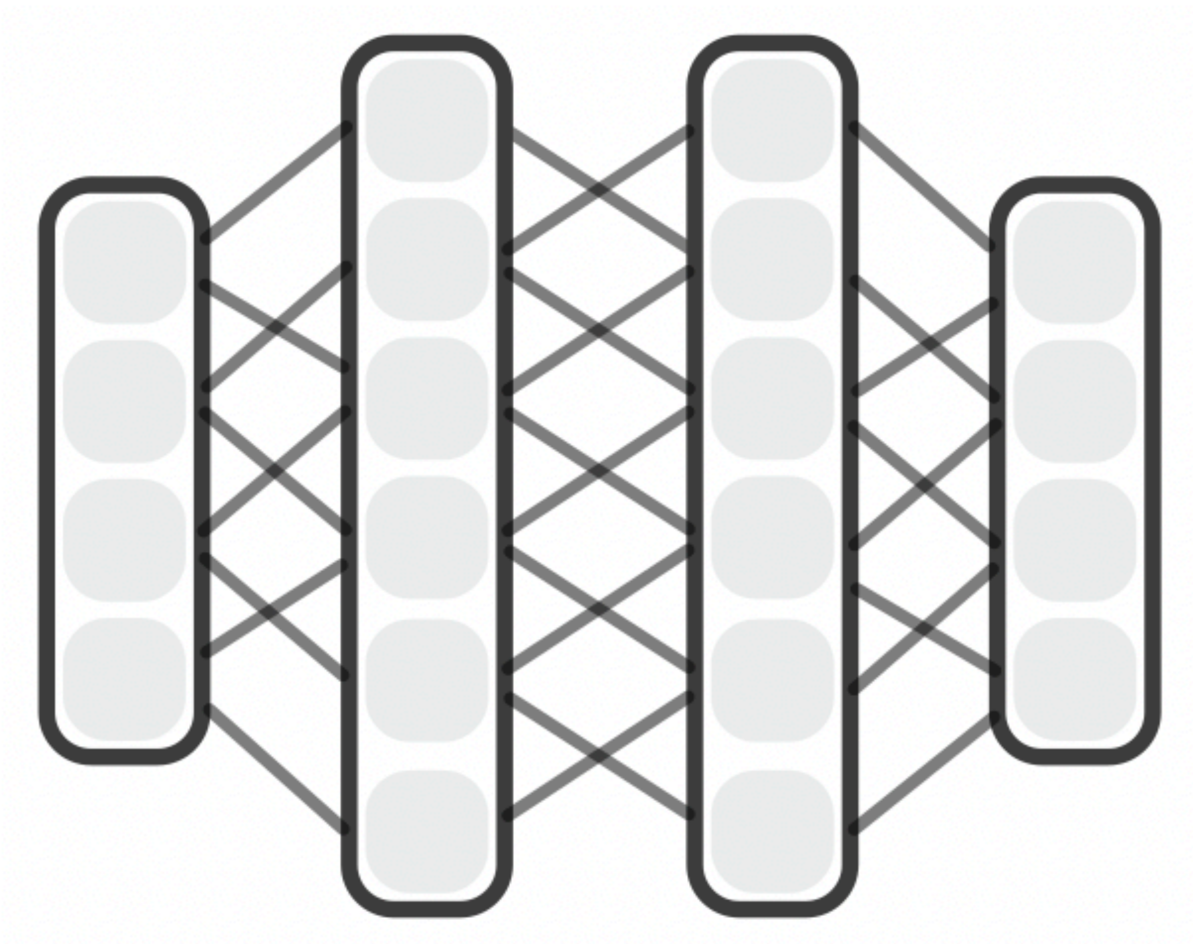
Neural Likelihood Estimation for the DDM

$\theta_i \rightarrow$



$\rightarrow x_j = \{r, c\}$

$\theta_i \rightarrow$



$\rightarrow q_\phi(r, c \,|\, \theta_i)$

Goals for SBI on DDMs

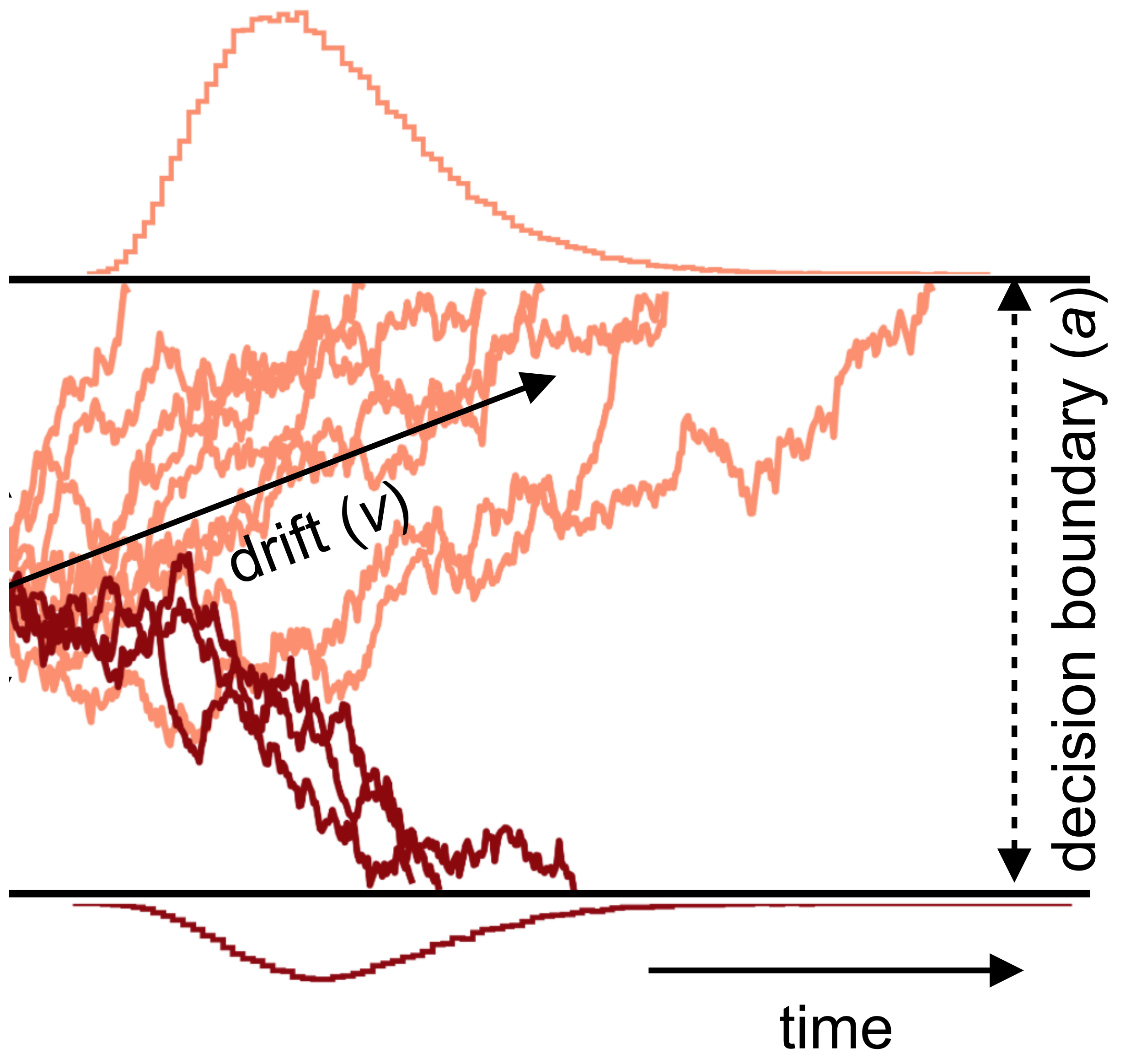
- Be efficient: few training simulations
- Be flexible: infer different numbers of trials

Advantage of NLE

Boelts et al. 2022

Neural Likelihood Estimation for the DDM

$\theta_i \rightarrow$



$\rightarrow x_j = \{r, c\}$

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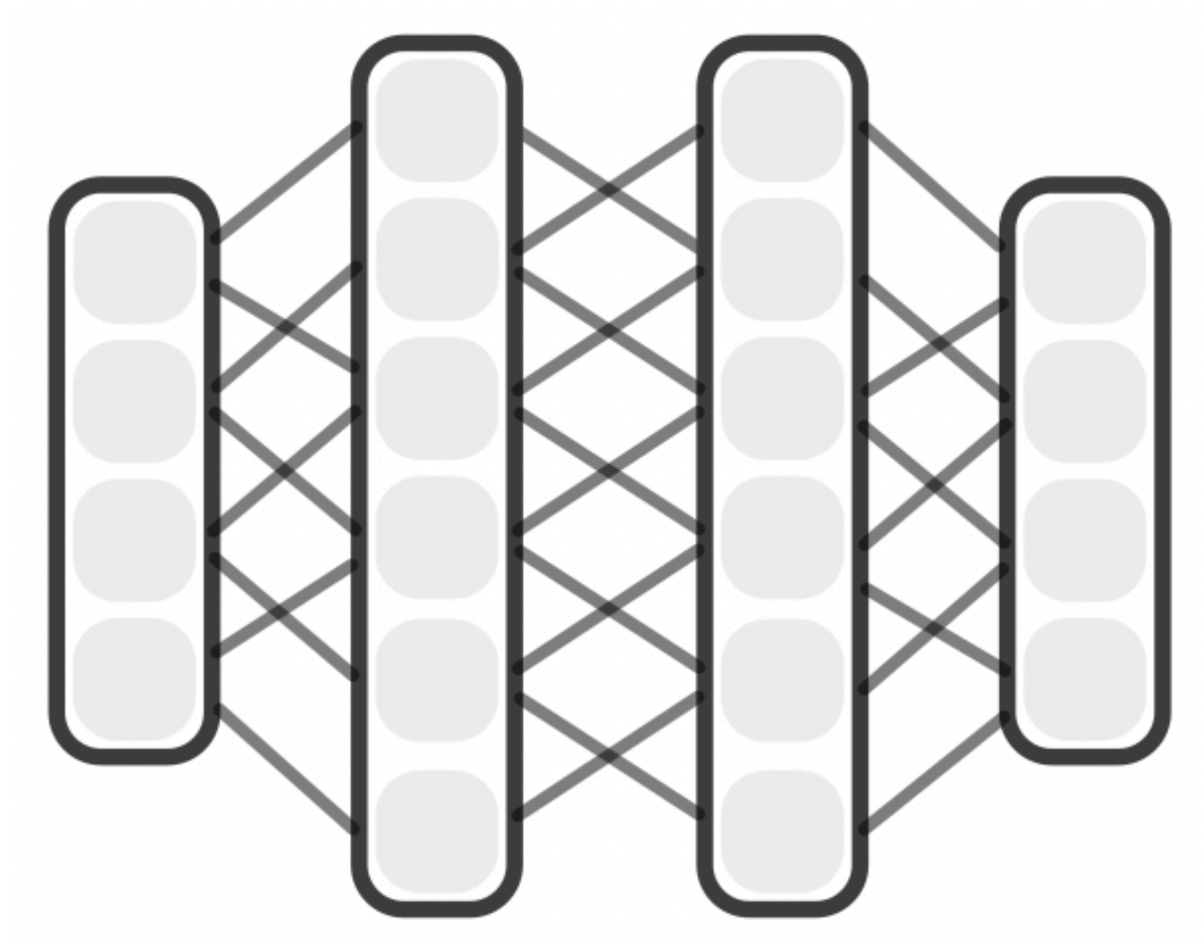


$\rightarrow q_\phi(r, c \mid \theta_i)$

Goals for SBI on DDMs

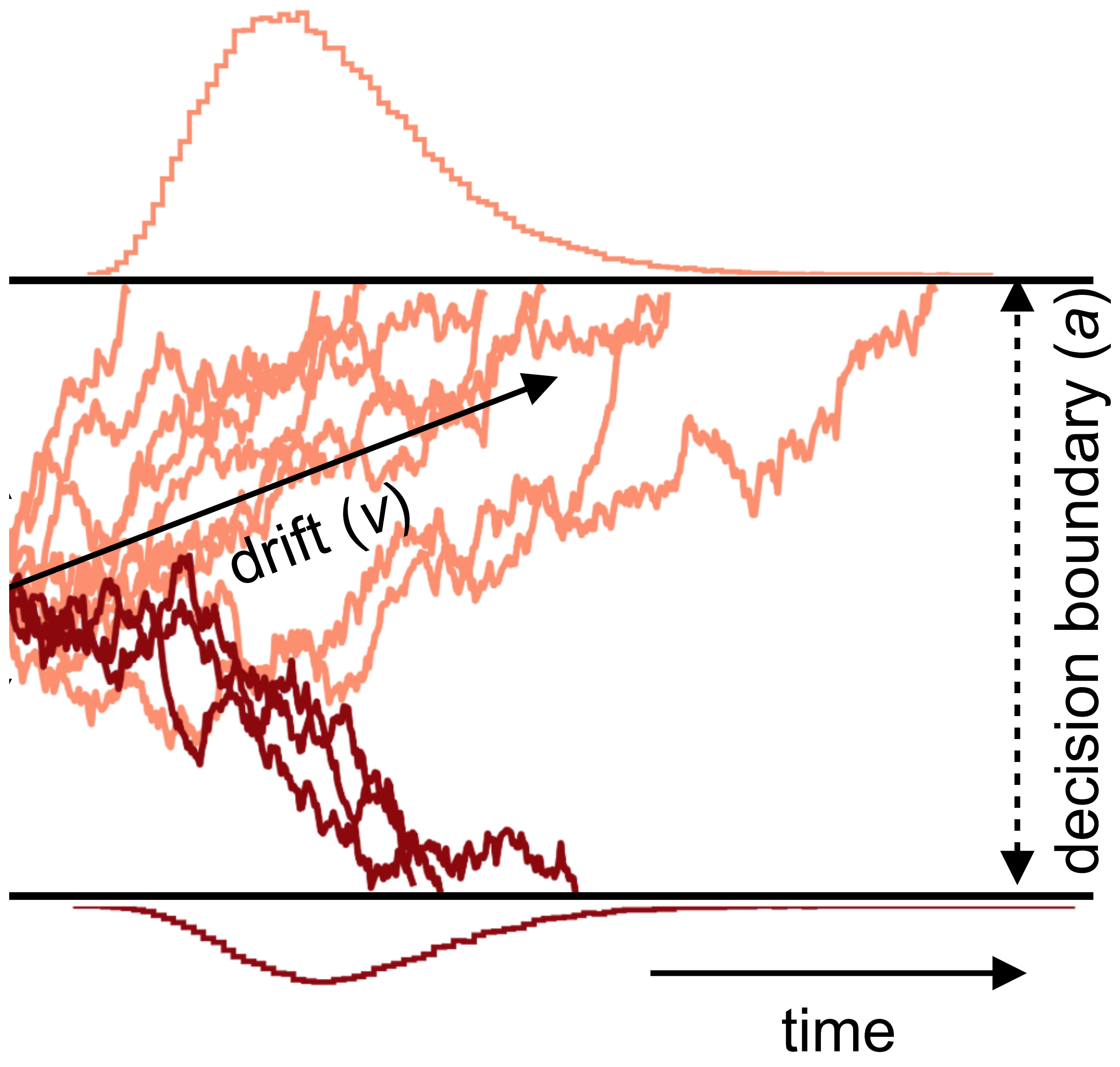
- Be efficient: few training simulations
- Be flexible: infer different numbers of trials

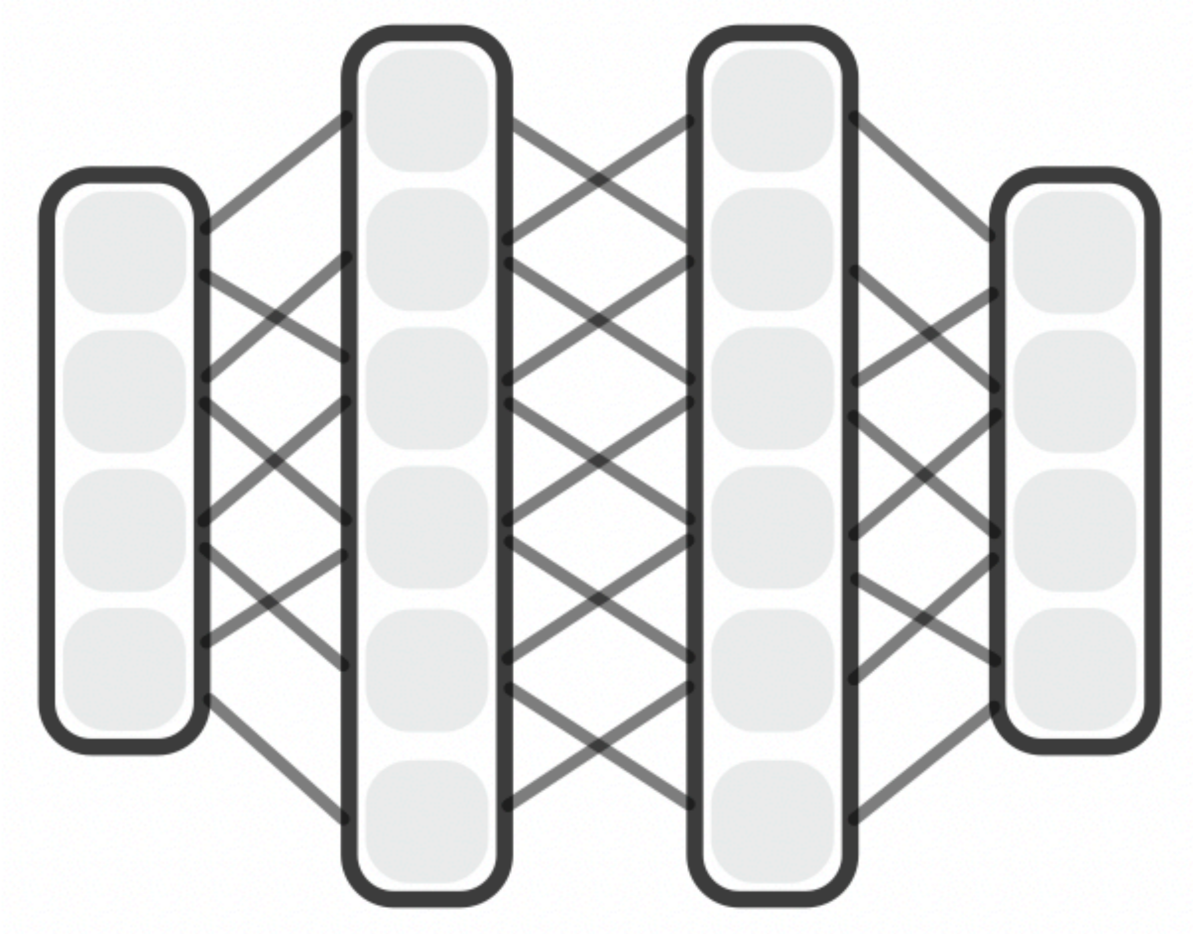
$$X_o = \{x_j\}_{i=1}^{M}$$

Advantage of NLE

Boelts et al. 2022

Neural Likelihood Estimation for the DDM

$\theta_i \rightarrow$  $\rightarrow x_j = \{r, c\}$

$\theta_i \rightarrow$  $\rightarrow q_\phi(r, c \mid \theta_i)$

Goals for SBI on DDMs

- Be efficient: few training simulations
- Be flexible: infer different numbers of trials

$$X_o = \{x_j\}_{i=1}^{M}$$

Advantage of NLE

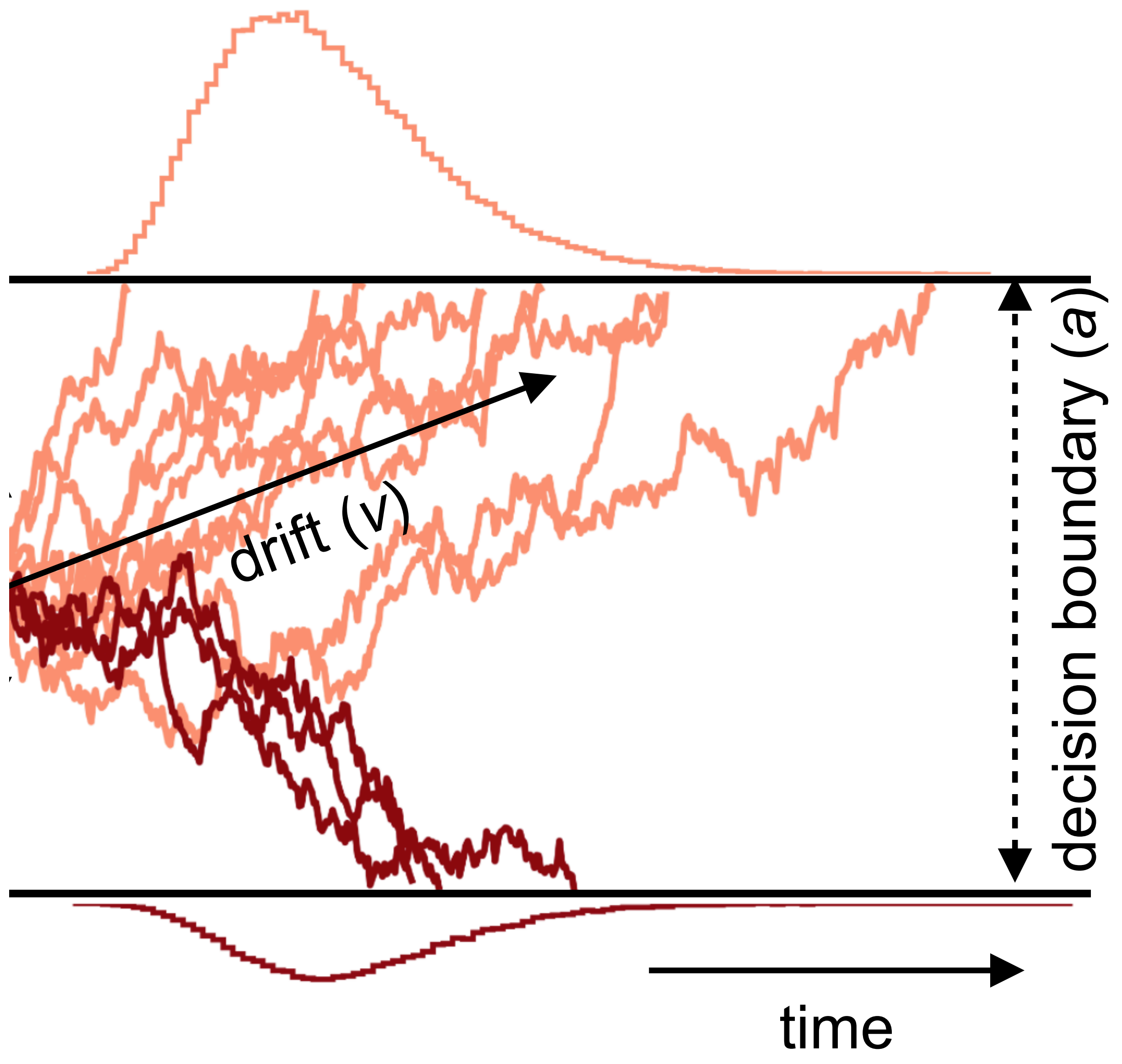
- train on single trials

$$x_j = \{r, c\}$$

Boelts et al. 2022

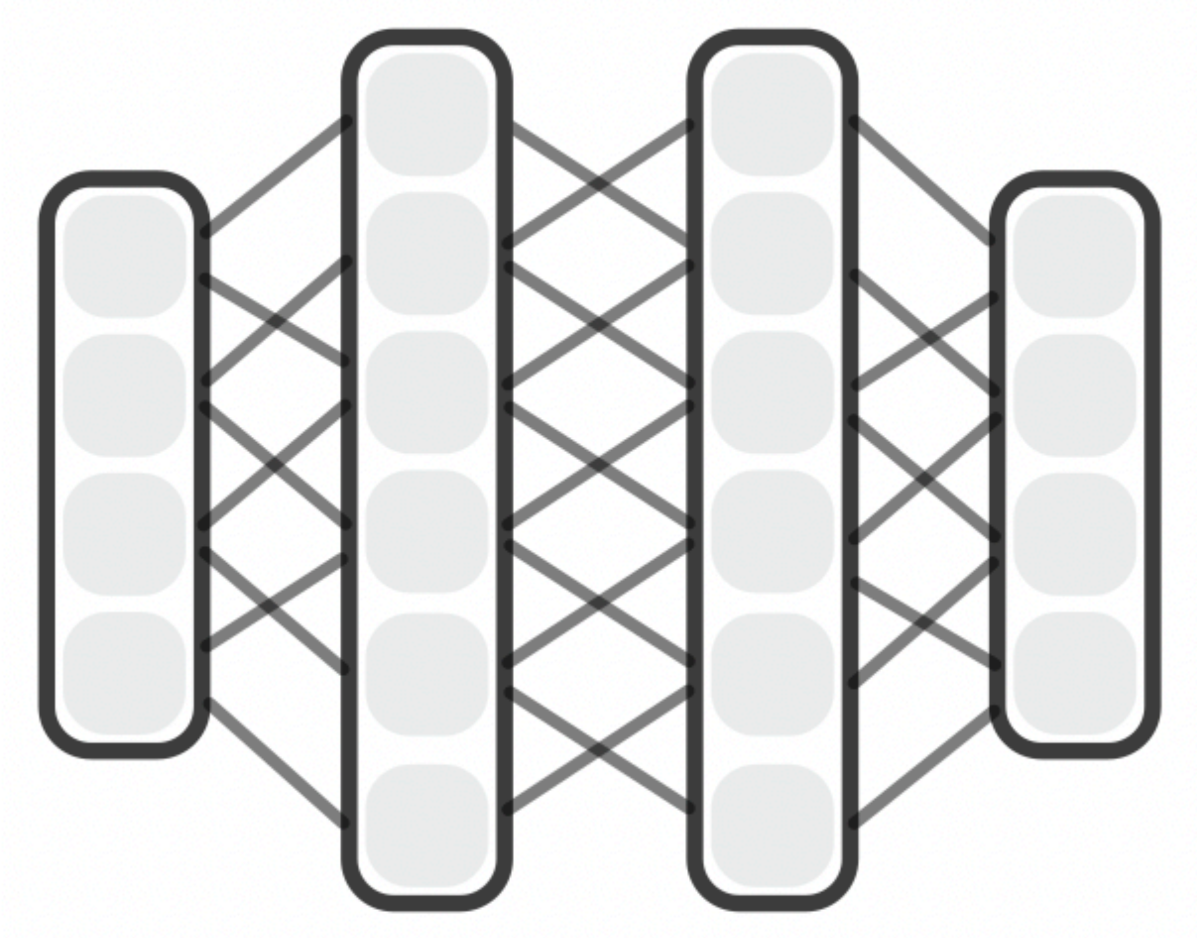
Neural Likelihood Estimation for the DDM

$\theta_i \rightarrow$



$\rightarrow x_j = \{r, c\}$

$\theta_i \rightarrow$



$\rightarrow q_\phi(r, c \,|\, \theta_i)$

Goals for SBI on DDMs

- Be efficient: few training simulations
- Be flexible: infer different numbers of trials

$$X_o = \{x_j\}_{i=1}^{M}$$

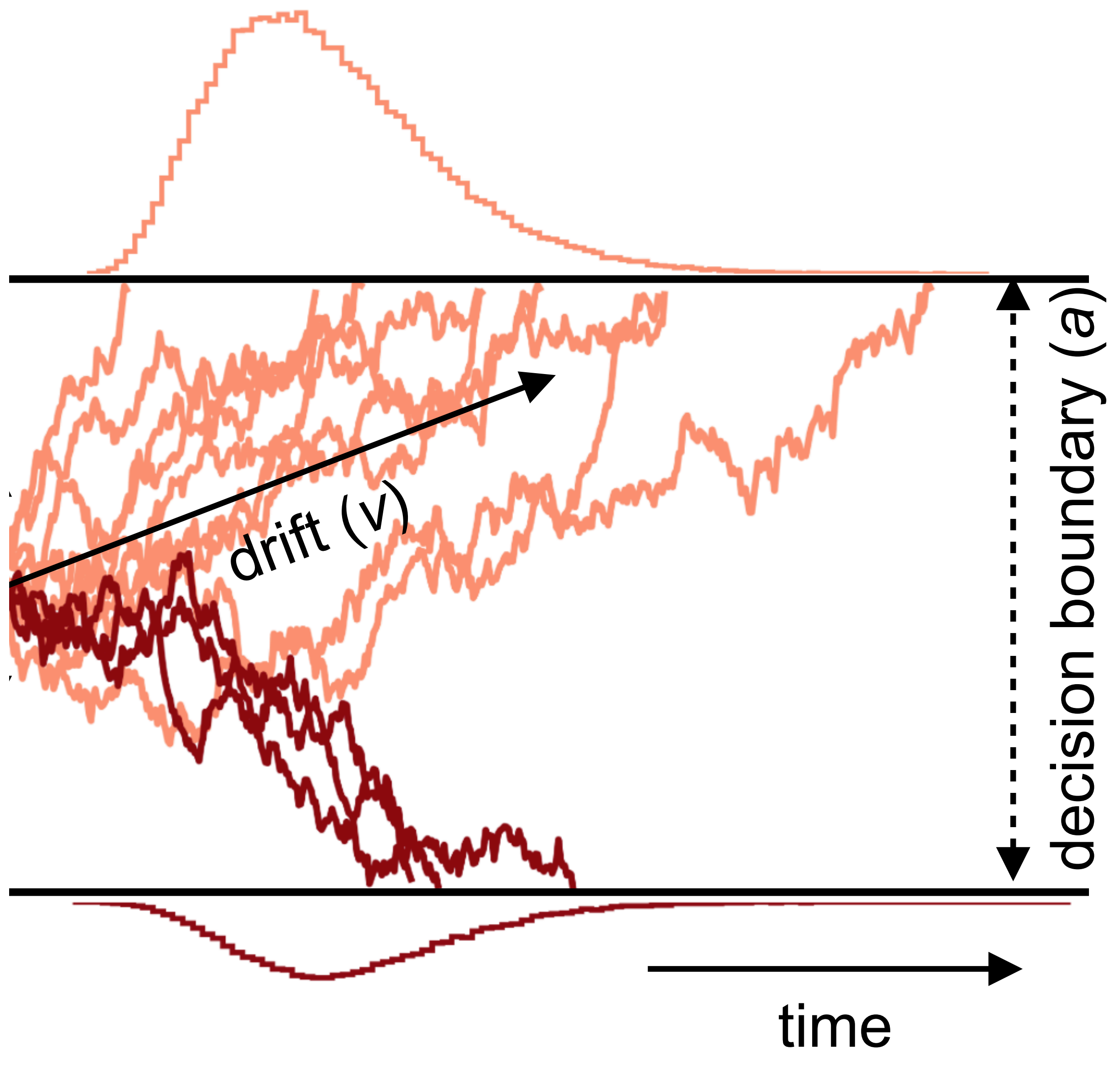
Advantage of NLE

- train on single trials $\quad x_j = \{r, c\}$
- inference with many trials $\quad q_\phi(X_o \,|\, \theta)$

Boelts et al. 2022

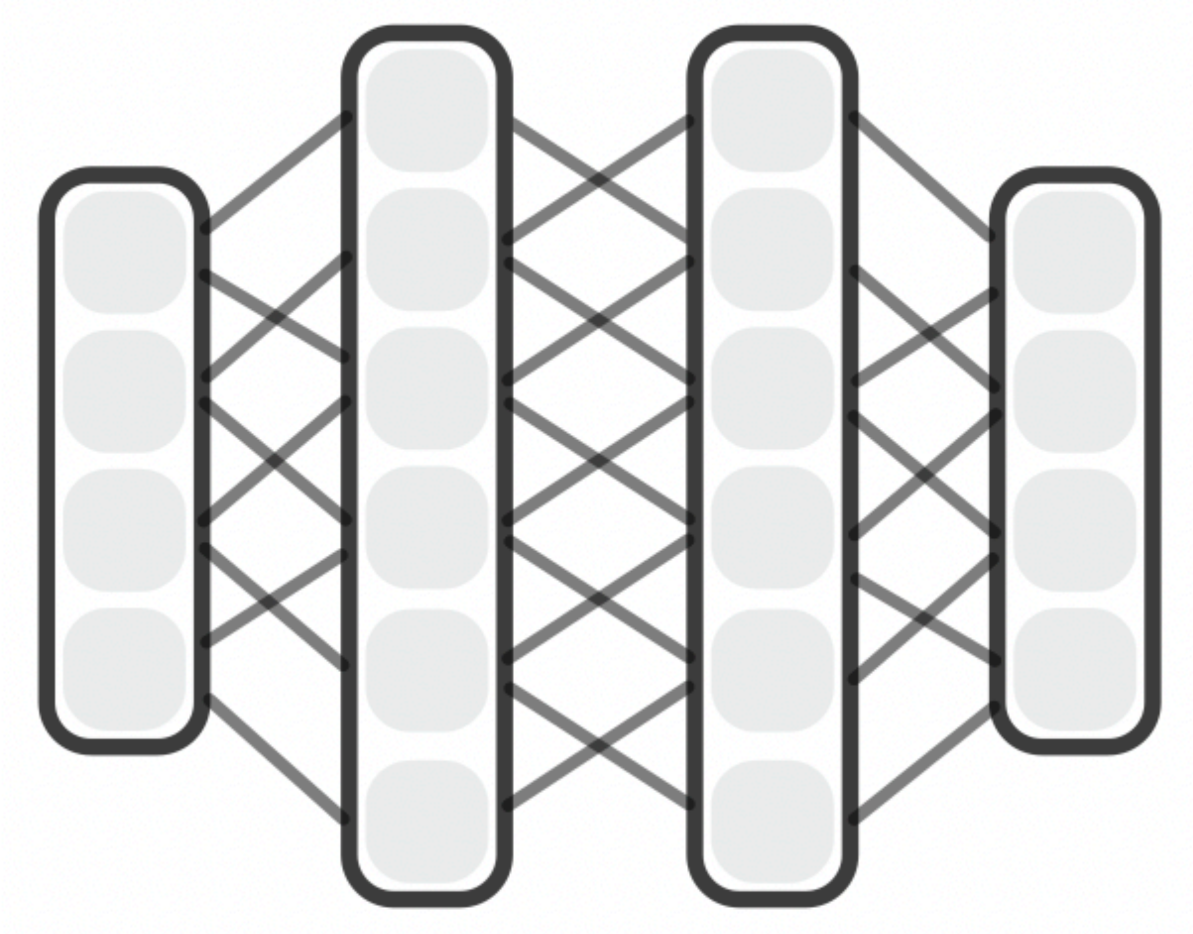
Neural Likelihood Estimation for the DDM

$\theta_i \rightarrow$



$\rightarrow x_j = \{r, c\}$

$\theta_i \rightarrow$



$\rightarrow q_\phi(r, c \mid \theta_i)$

Goals for SBI on DDMs

- Be efficient: few training simulations
- Be flexible: infer different numbers of trials

$$X_o = \{x_j\}_{i=1}^{M}$$

Advantage of NLE

- train on single trials $\quad x_j = \{r, c\}$
- inference with many trials $\quad q_\phi(X_o \mid \theta)$
- assume trials are independent: $\quad \prod_{j=1}^{M} q_\phi(x_j \mid \theta)$

  "i.i.d.-assumption"

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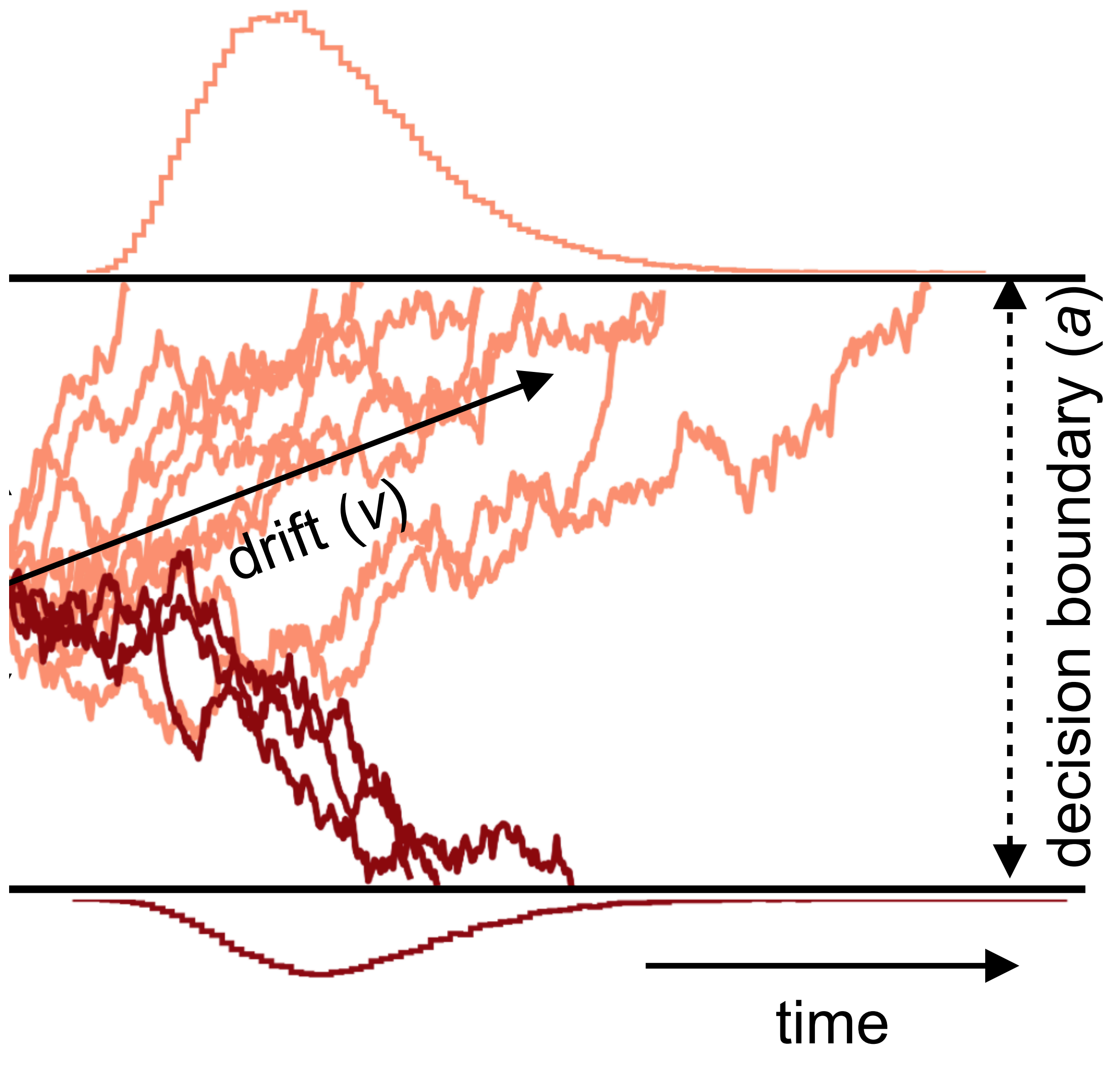
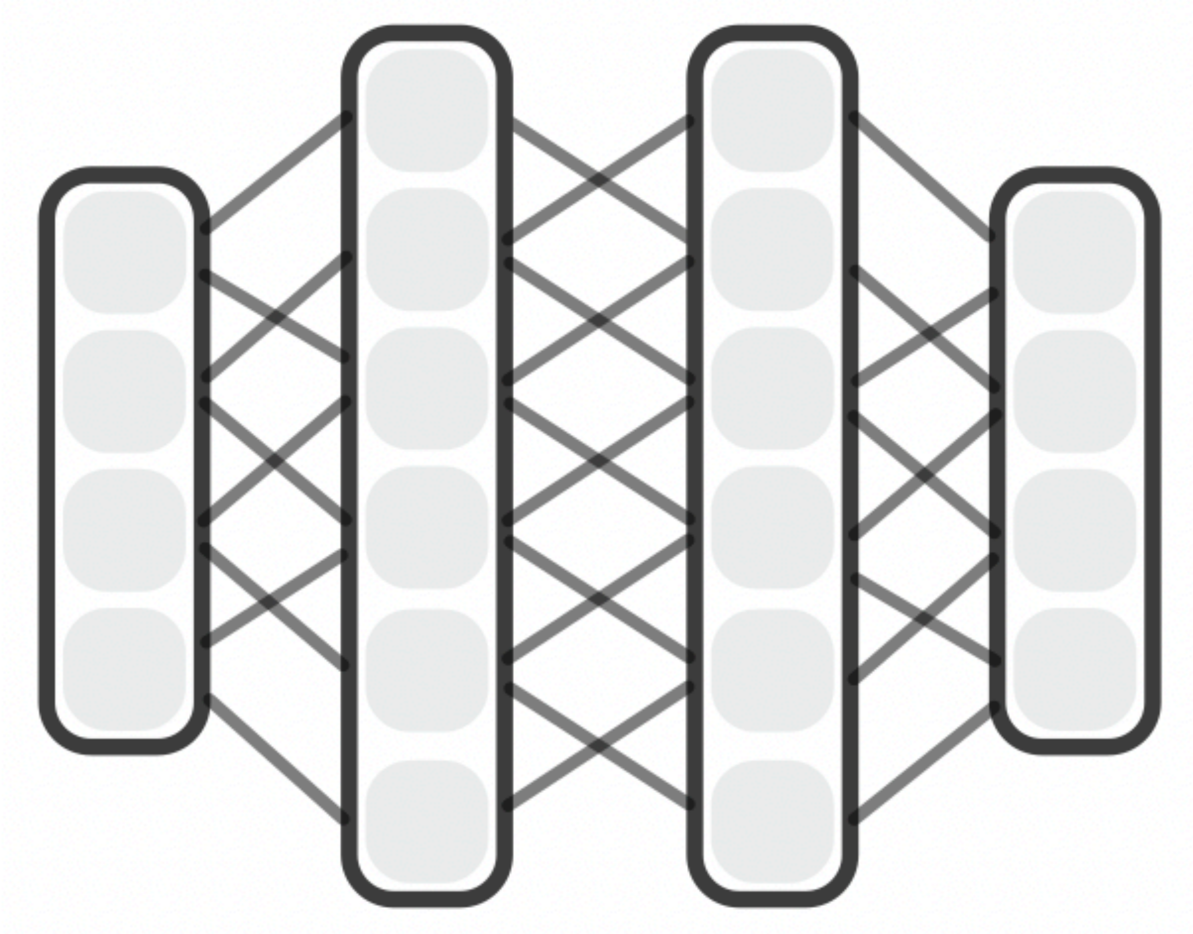
Neural Likelihood Estimation for the DDM

$\theta_i \rightarrow$



$\rightarrow x_j = \{r, c\}$

$\theta_i \rightarrow$



$\rightarrow q_\phi(r, c \mid \theta_i)$

Challenge

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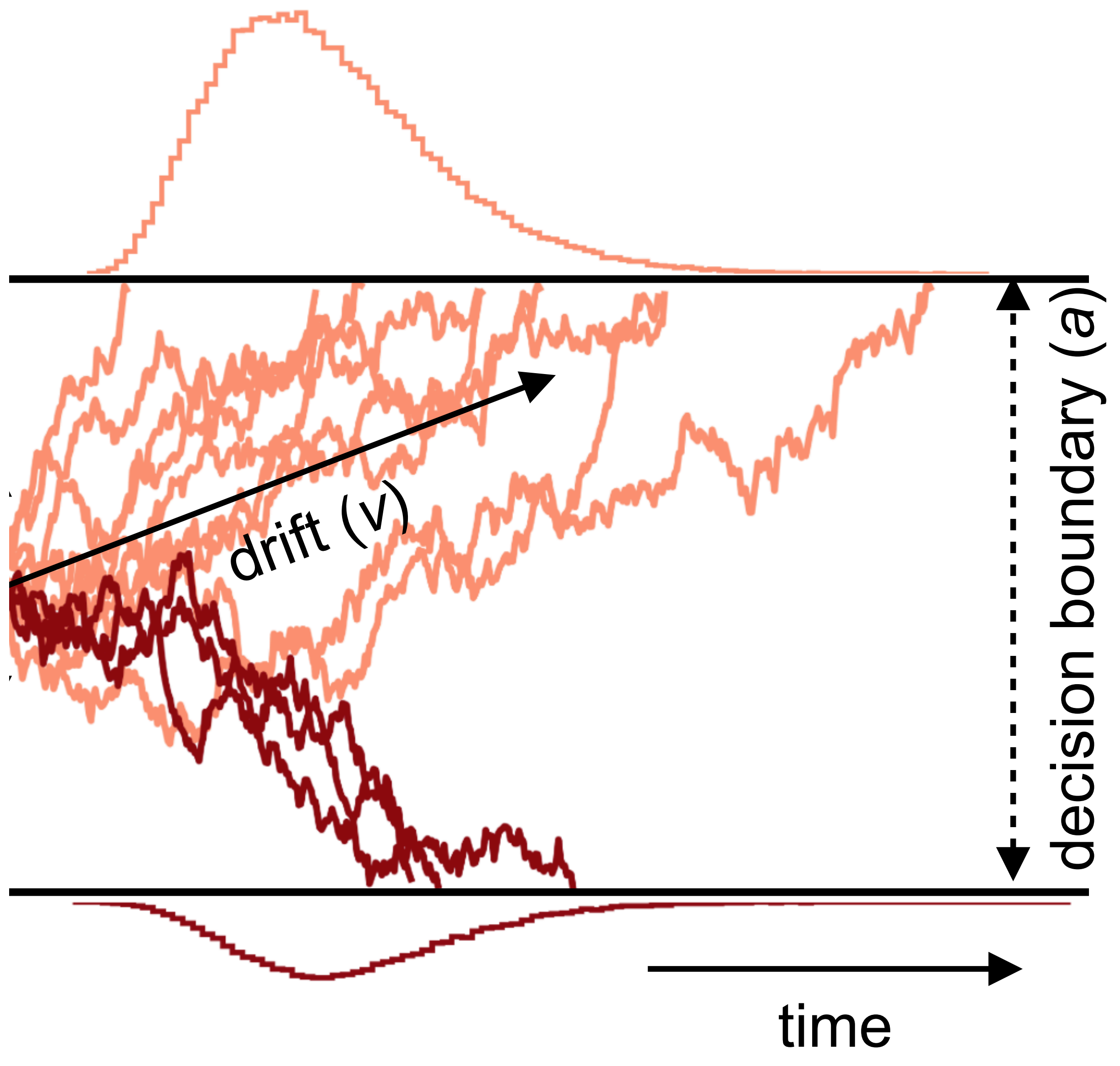
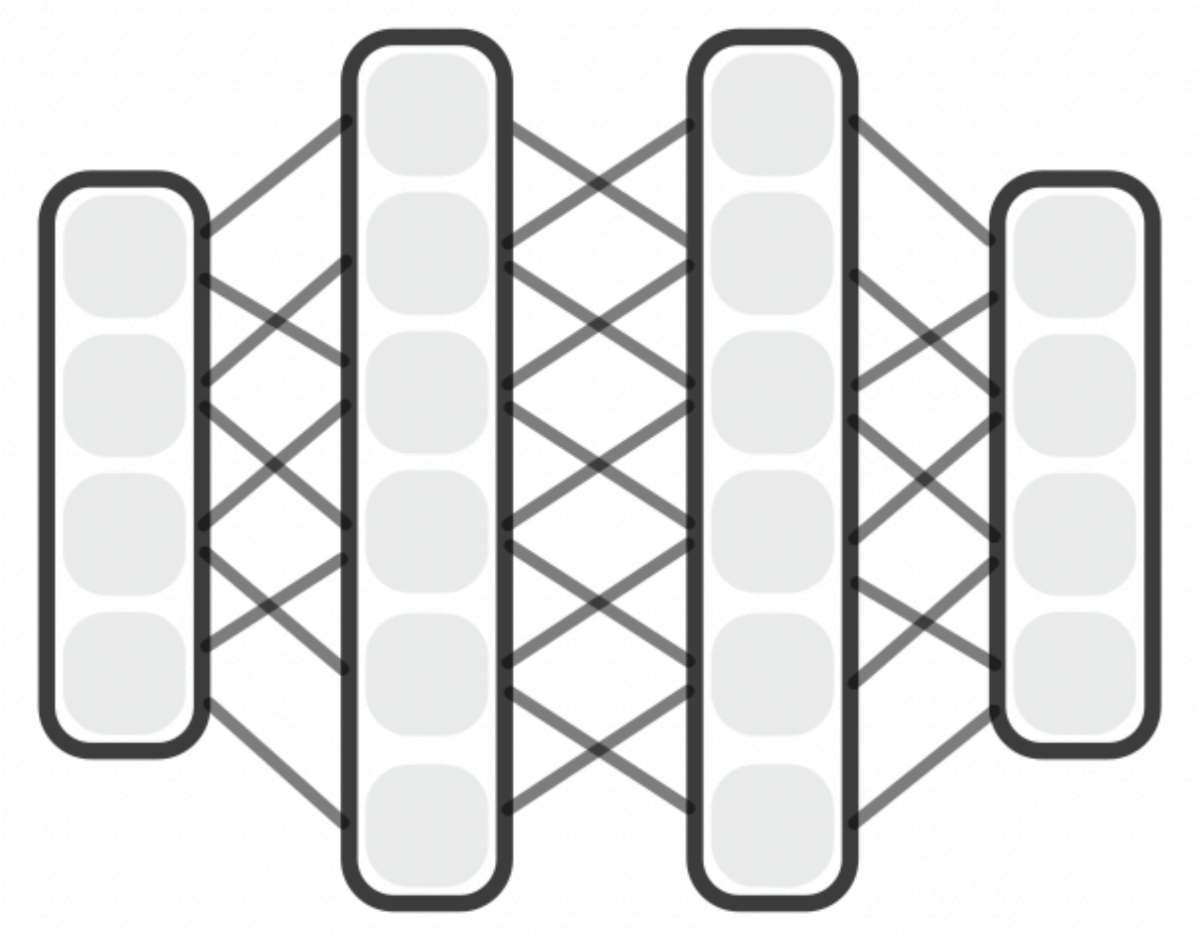
Neural Likelihood Estimation for the DDM

$\theta_i \rightarrow$ 

$\rightarrow x_j = \{r, c\}$

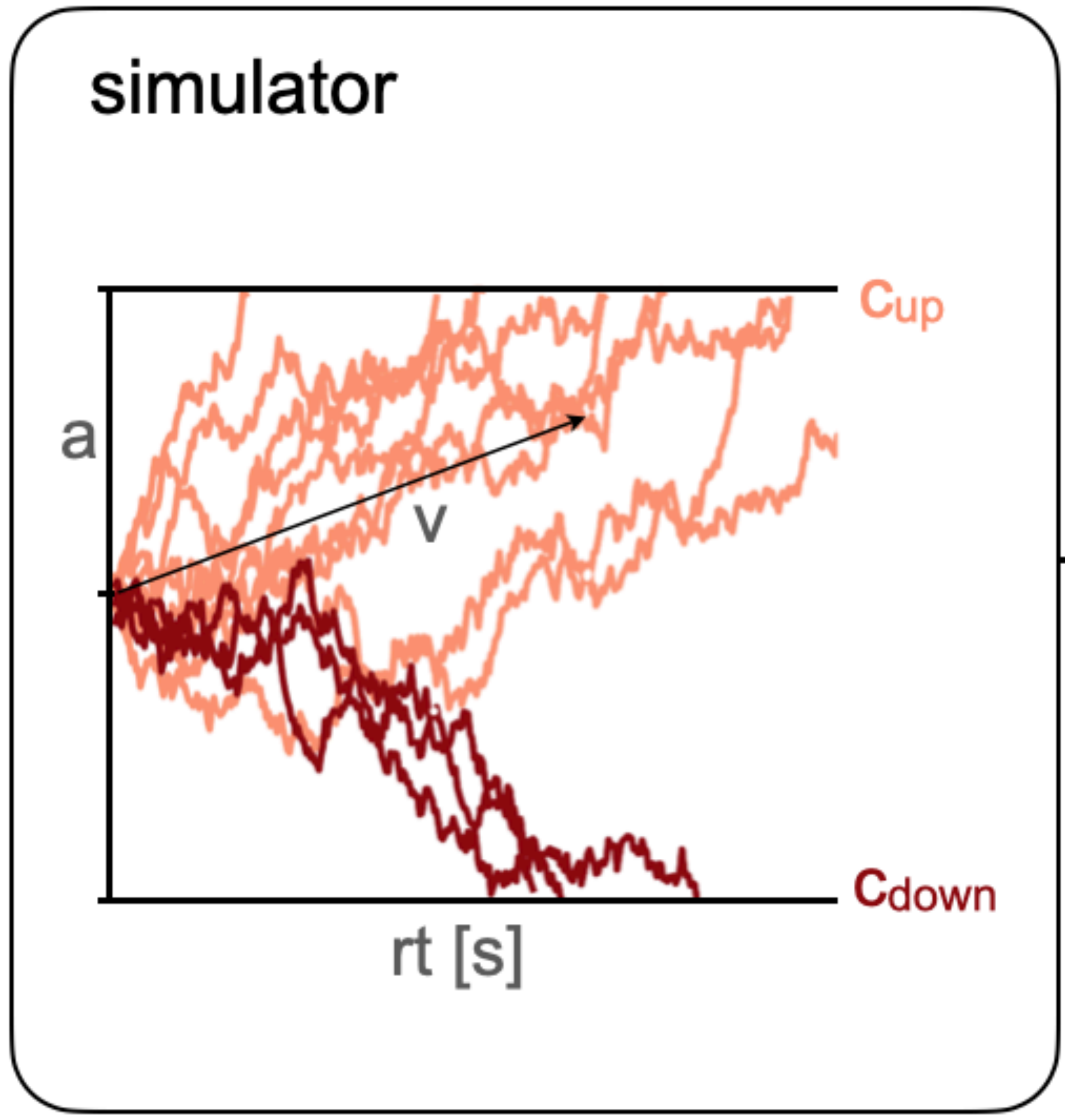
$\theta_i \rightarrow$  $\rightarrow q_\phi(r, c \mid \theta_i)$

Challenge

- Density estimation for mixed data
- $r \in \mathbb{R} \quad c \in \mathbb{N}$
- **continuous** reaction times (time)
- **discrete** choices (left, right)

Boelts et al. 2022

Mixed Neural Likelihood Estimation (MNLE)



Solution:

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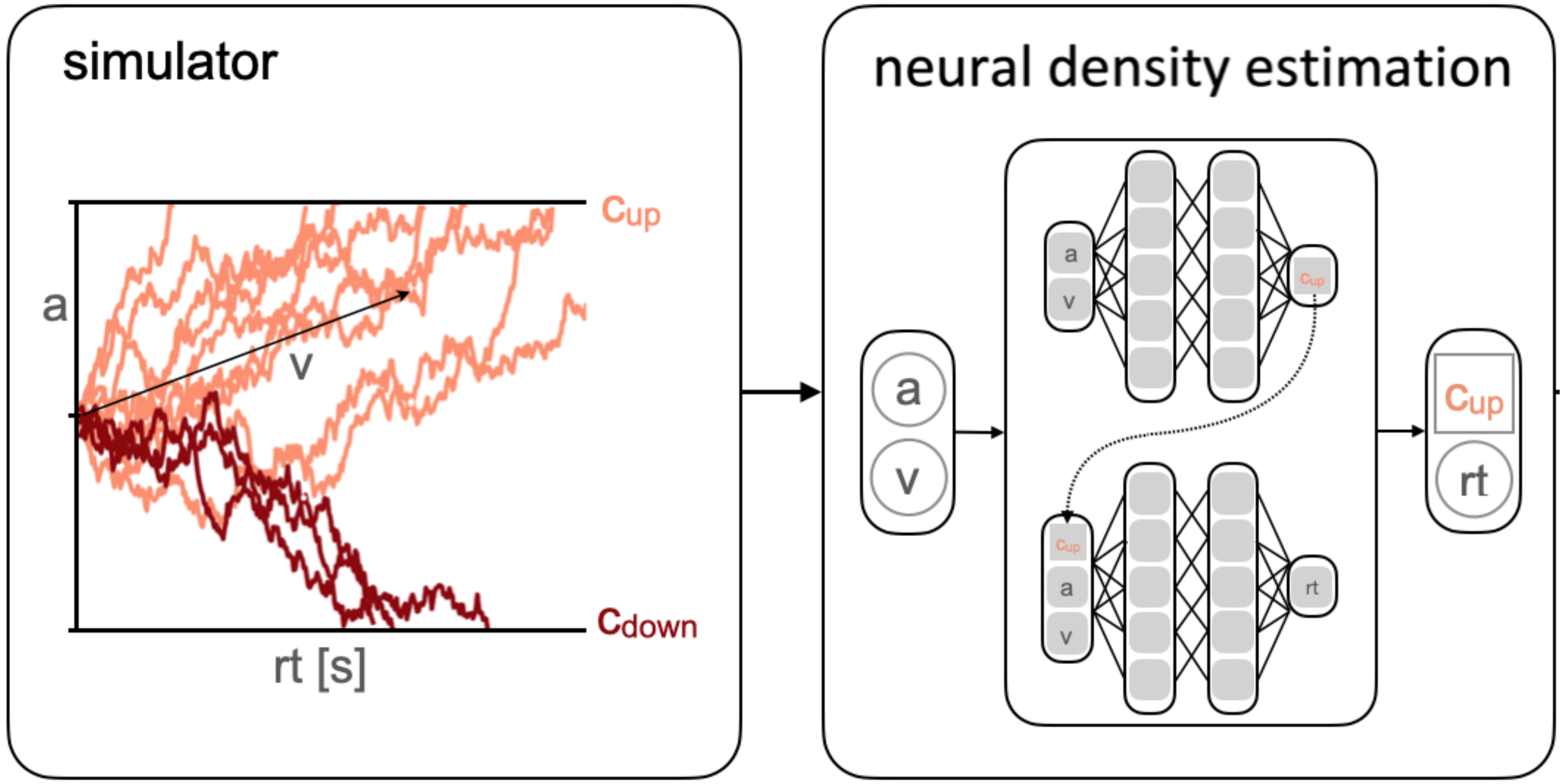
Mixed Neural Likelihood Estimation (MNLE)

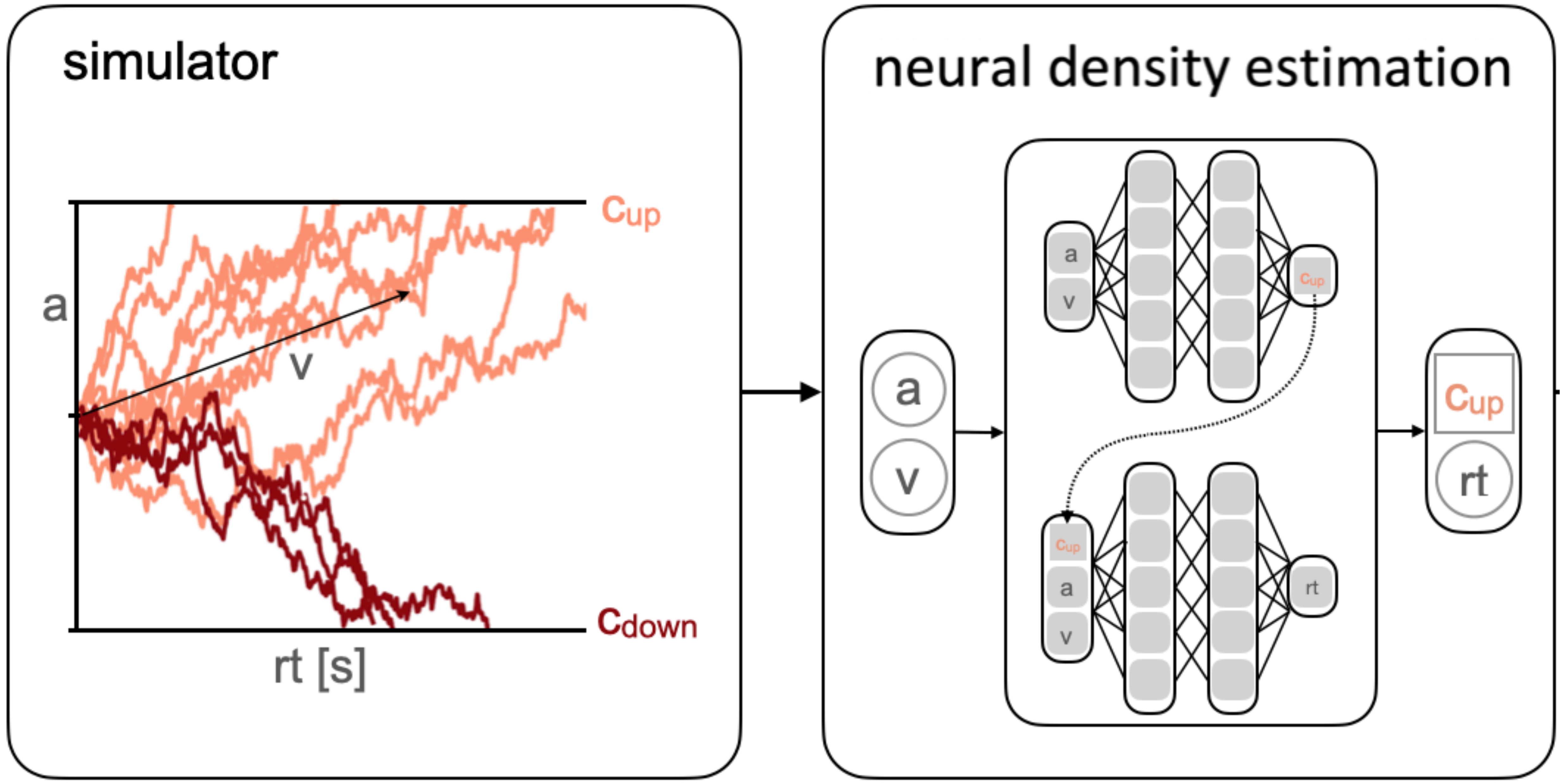


Solution:

- Learn separate density estimators for r and c: $$q(r, c \,|\, \theta) = \underbrace{q_\psi(c \,|\, \theta)\; q_\phi(r \,|\, c, \theta)}$$

Boelts et al. 2022

Mixed Neural Likelihood Estimation (MNLE)

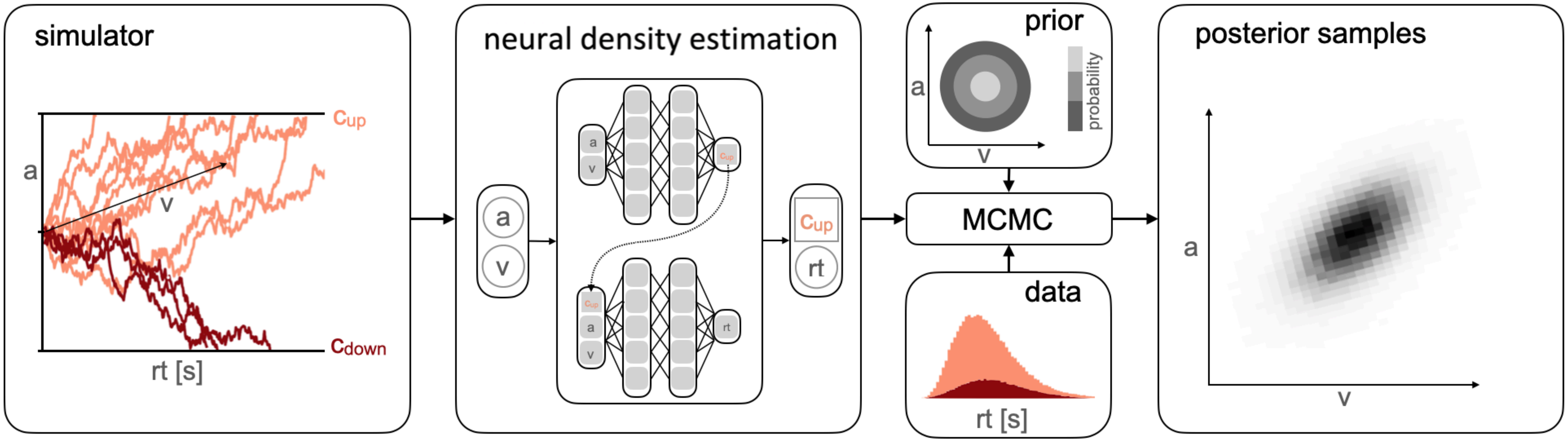


Solution:

- Learn separate density estimators for r and c: $q(r, c \mid \theta) = q_{\psi}(c \mid \theta)\, q_{\phi}(r \mid c, \theta)$
- Combine likelihood estimators for inference: $p(\theta \mid r, c) \propto q(r, c \mid \theta) p(\theta)$

Boelts et al. 2022

Mixed Neural Likelihood Estimation (MNLE)



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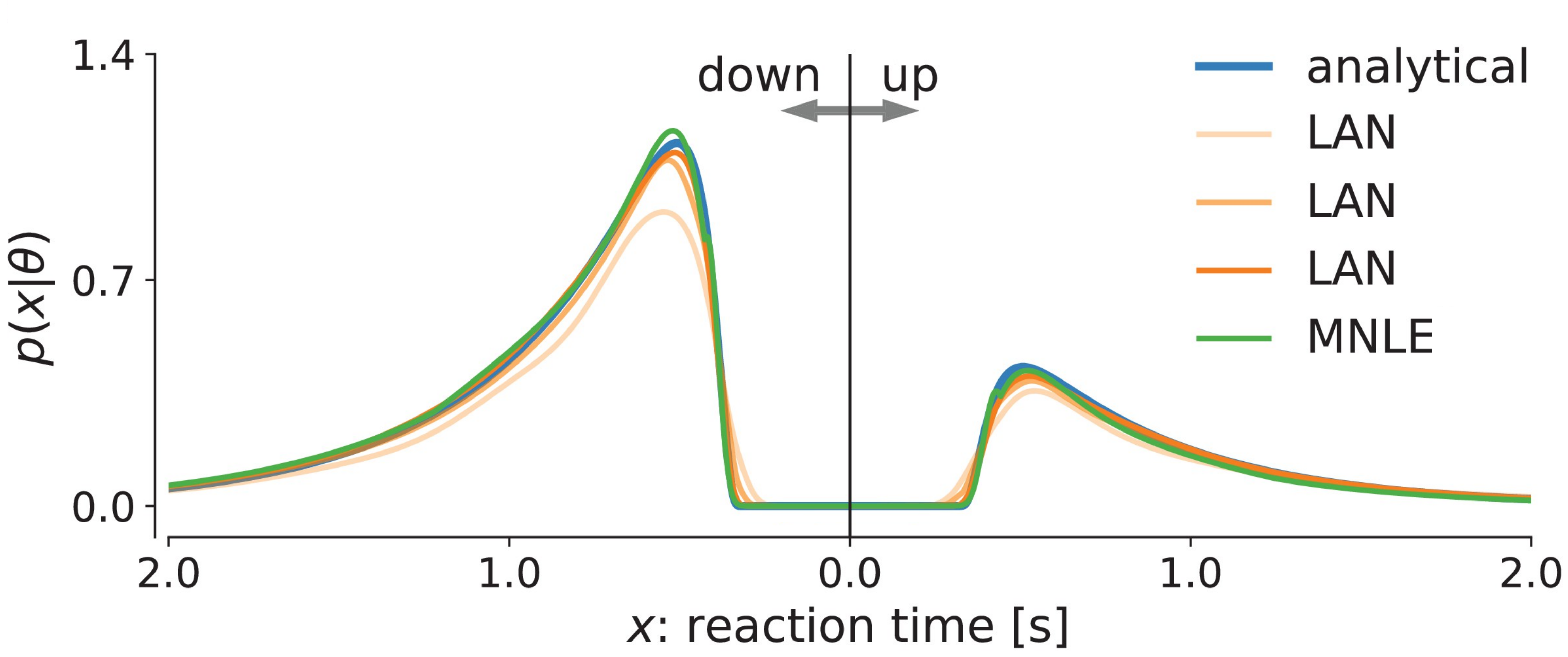
Boelts et al. 2022

MNLE is accurate and efficient

Boelts et al. 2022; Fengler et al. 2021

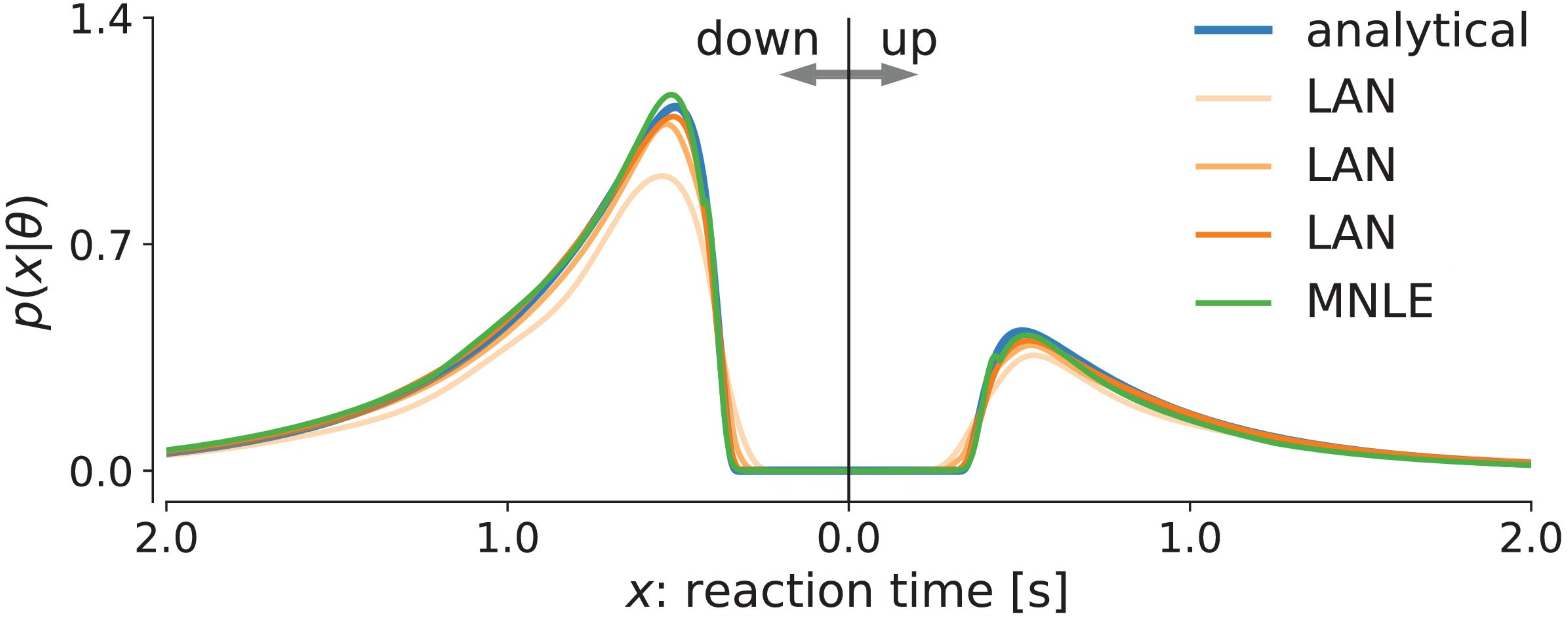
MNLE is accurate and efficient



Compare likelihood accuracy of MNLE:

Boelts et al. 2022; Fengler et al. 2021

MNLE is accurate and efficient

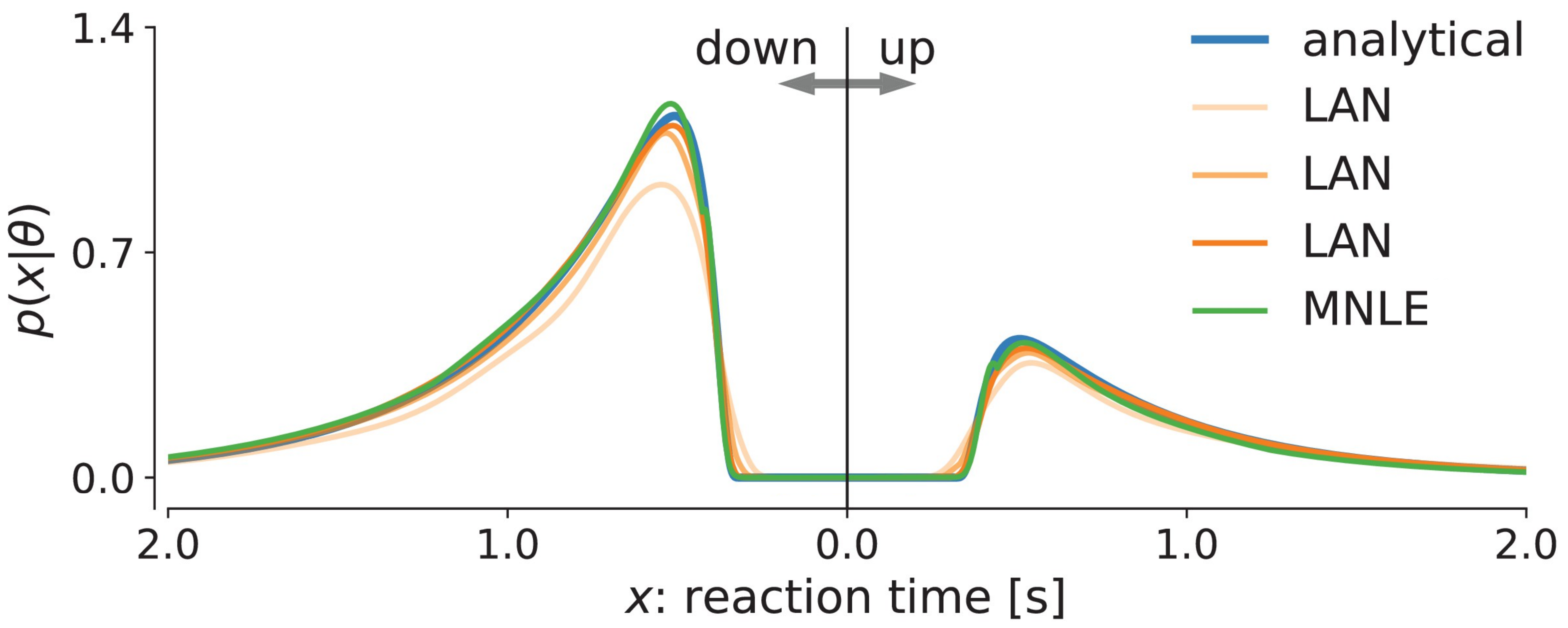


Compare likelihood accuracy of MNLE:

- analytical solution

Boelts et al. 2022; Fengler et al. 2021

MNLE is accurate and efficient

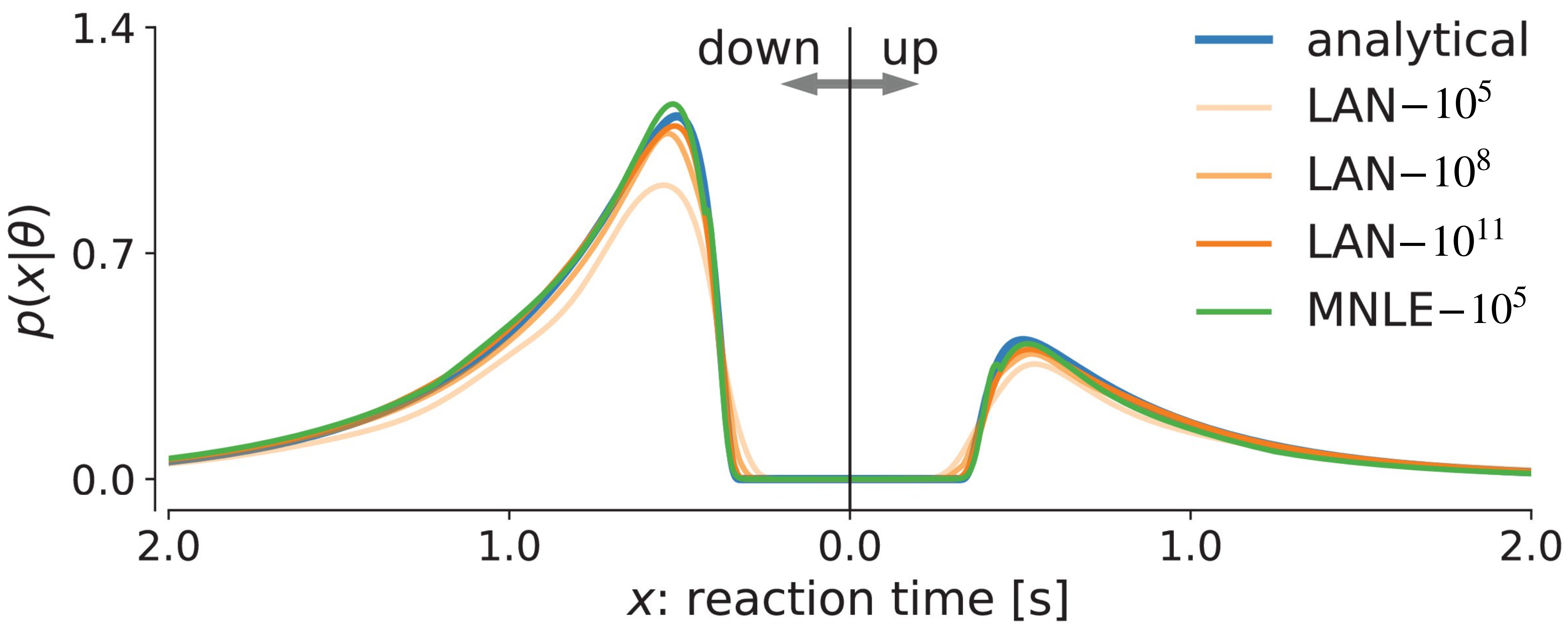


Compare likelihood accuracy of MNLE:

- analytical solution
- Likelihood Approximation Networks (LAN)

Boelts et al. 2022; Fengler et al. 2021

MNLE is accurate and efficient



Compare likelihood accuracy of MNLE:

- analytical solution
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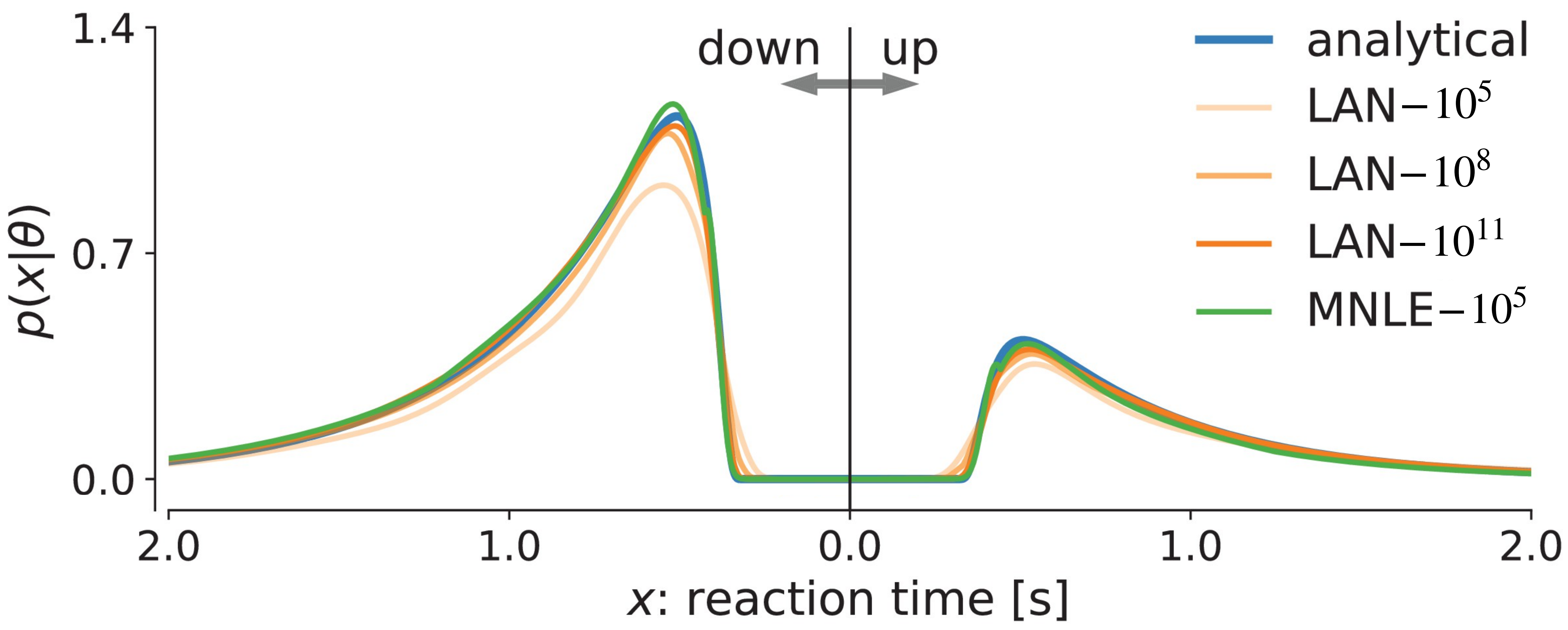
Compare simulation efficiency

Boelts et al. 2022; Fengler et al. 2021

MNLE is accurate and efficient



Compare likelihood accuracy of MNLE:

- analytical solution
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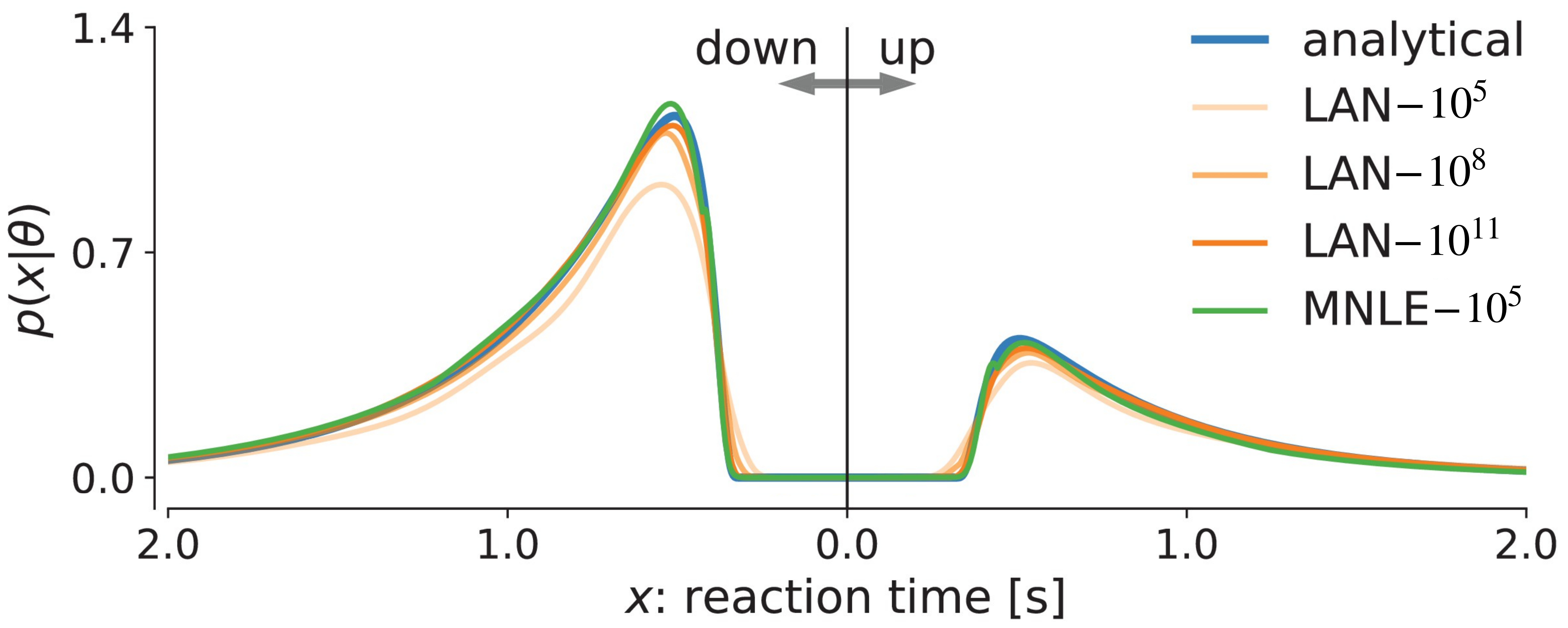
Compare simulation efficiency

- MNLE needs 100,000 simulations 🔥

Boelts et al. 2022; Fengler et al. 2021

MNLE is accurate and efficient



Compare likelihood accuracy of MNLE:

- analytical solution
- Likelihood Approximation Networks (LAN)

Compare simulation efficiency

- MNLE needs 100,000 simulations 🔥
- LAN needs 100,000,000,000 simulations 🤯

Boelts et al. 2022; Fengler et al. 2021

MNLE gives accurate posterior samples

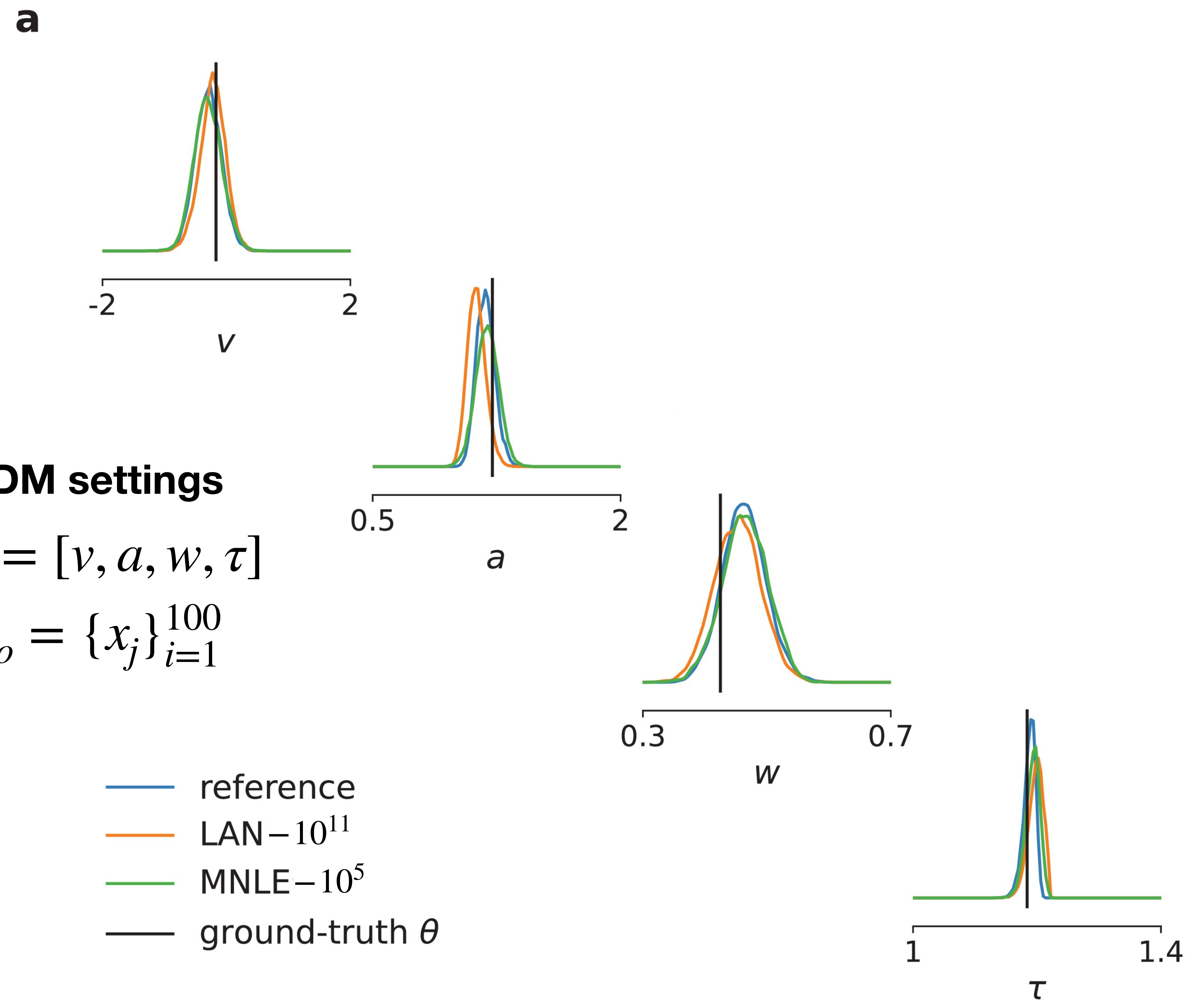
DDM settings

$\theta = [v, a, w, \tau]$

$X_o = \{x_j\}_{i=1}^{100}$

Boelts et al. 2022

MNLE gives accurate posterior samples



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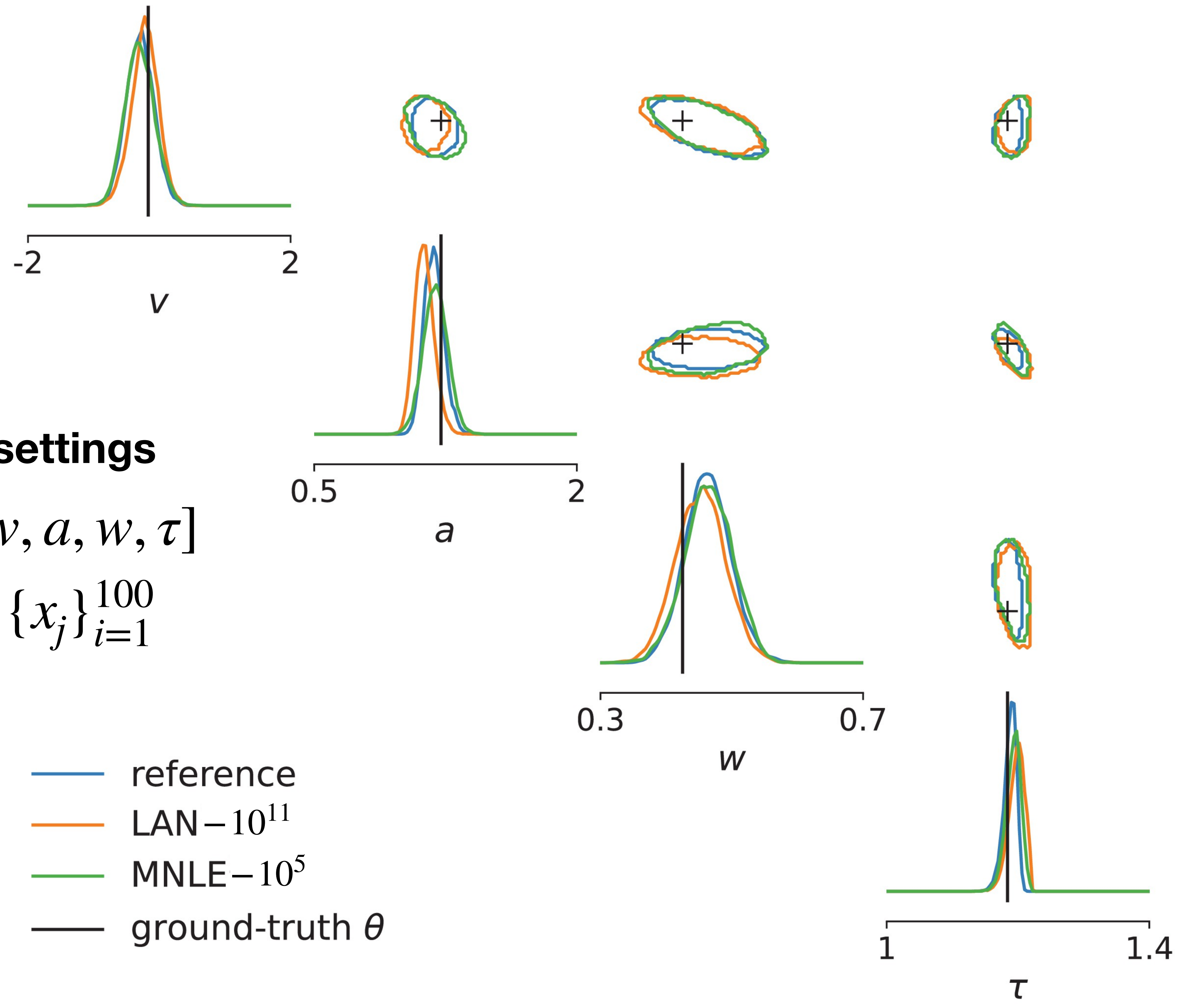
Boelts et al. 2022

MNLE gives accurate posterior samples

a



DDM settings

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Boelts et al. 2022

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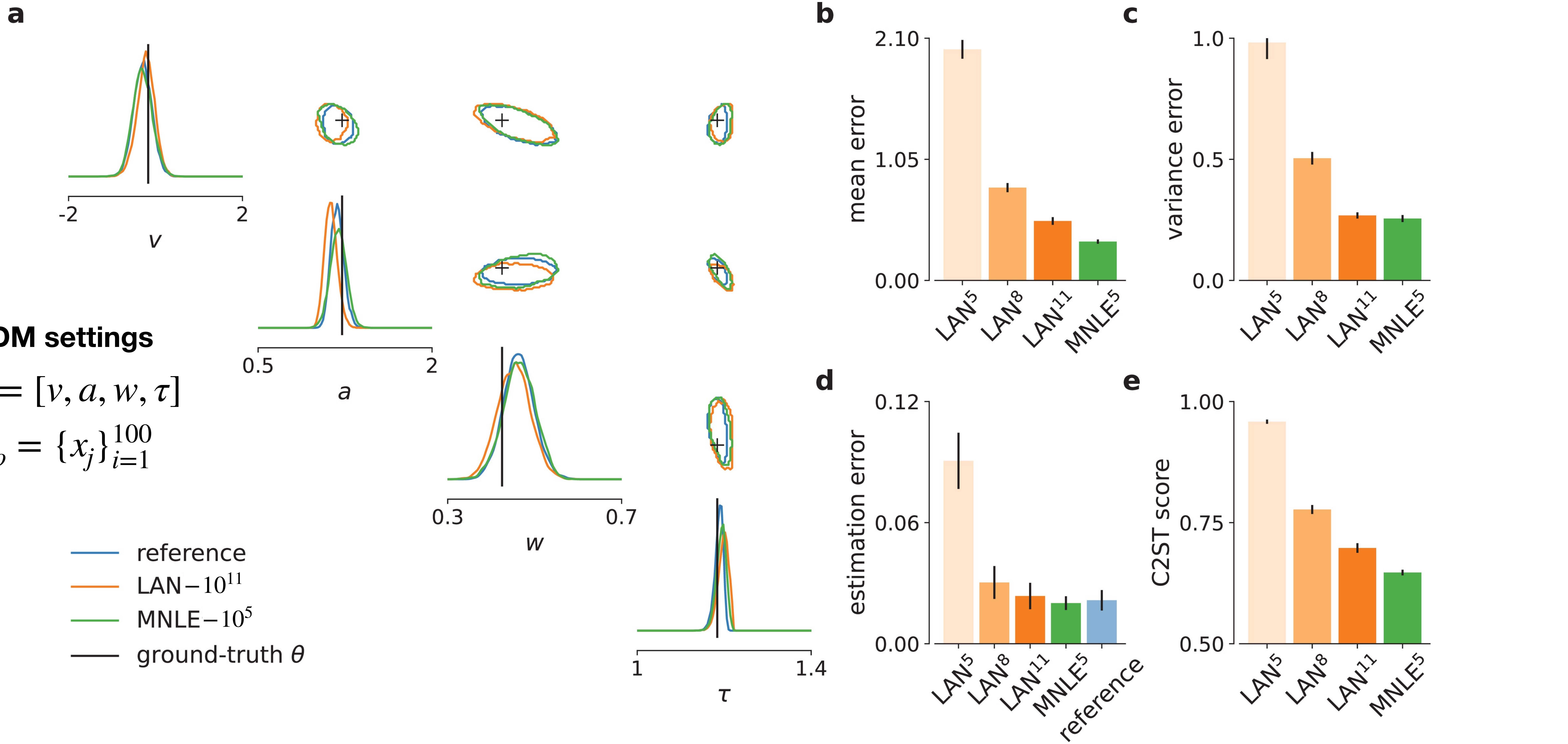

DDM settings

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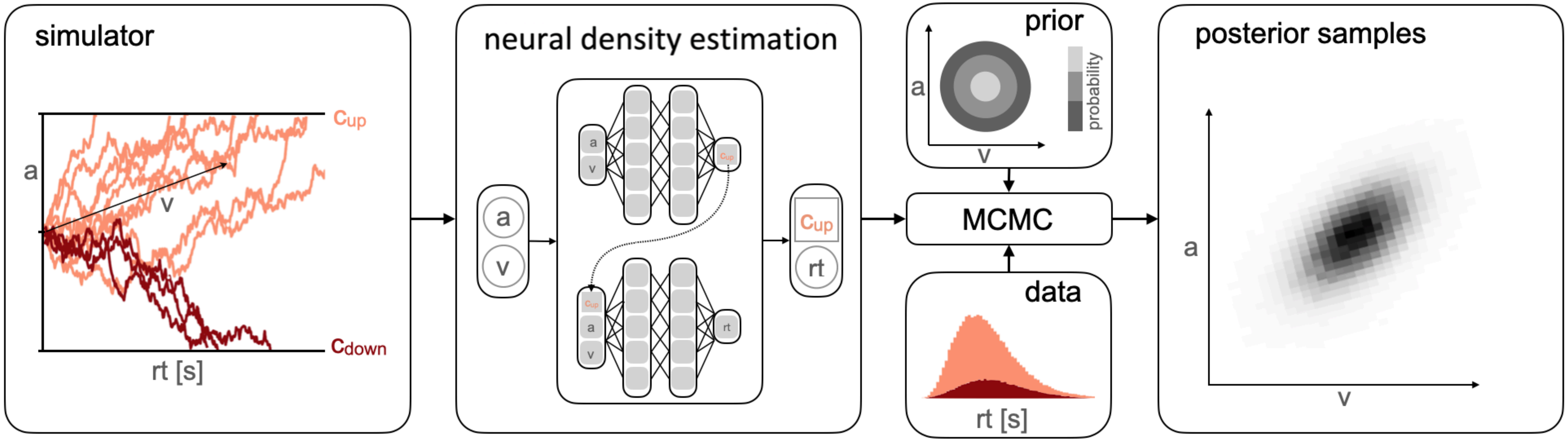
Boelts et al. 2022

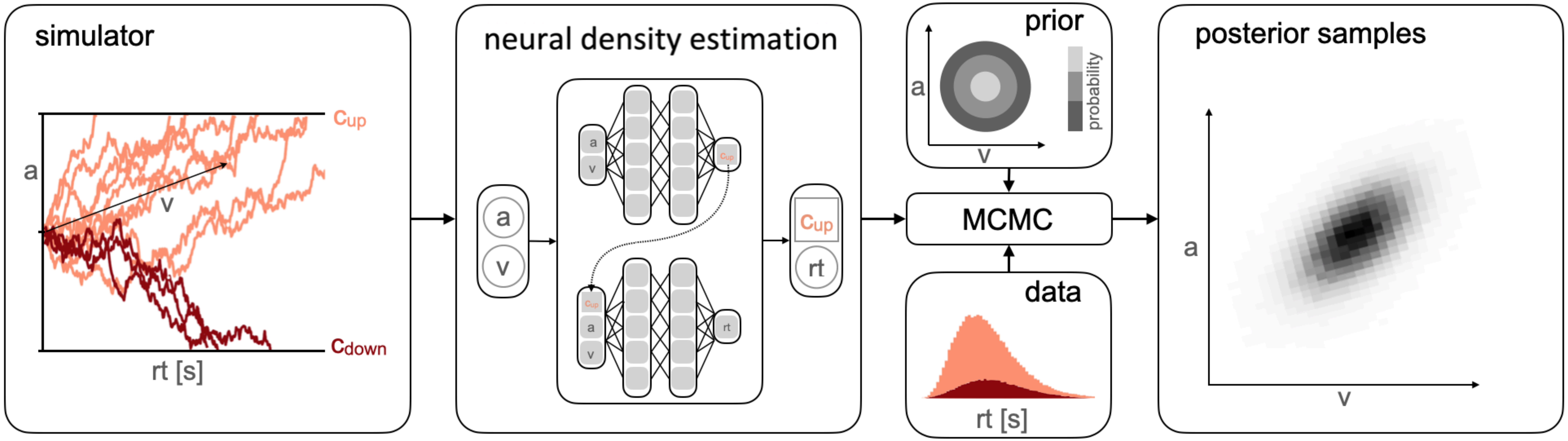
Summary: SBI for decision-making research



- MNLE enables SBI for simulators with mixed data

Boelts et al. 2022

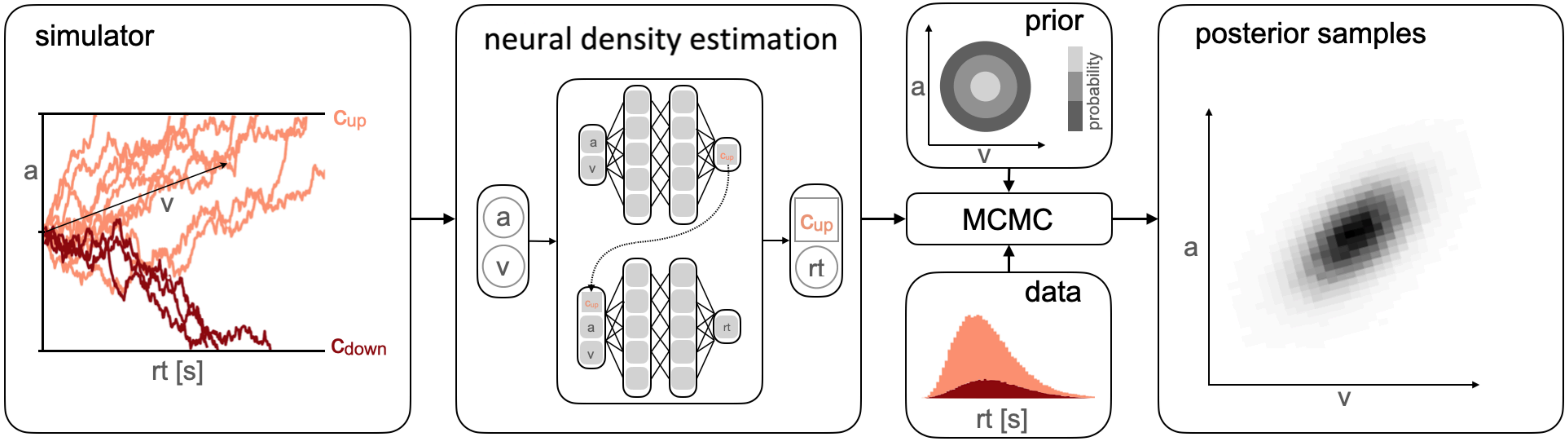
Summary: SBI for decision-making research



- MNLE enables SBI for simulators with mixed data
- Ideal for decision-making research with many-trial data

Boelts et al. 2022

Summary: SBI for decision-making research



- MNLE enables SBI for simulators with mixed data
- Ideal for decision-making research with many-trial data
- High simulation efficiency: inference beyond canonical DDMs

Boelts et al. 2022

Advancing Methods and Applicability of SBI in neuroscience

1. A new SBI method for **decision-making research** ✓
2. How to apply SBI in **Connectomics**
3. Software tools and guidelines for SBI

Advancing Methods and Applicability of SBI in neuroscience

1. A new SBI method for **decision-making research** ✓

2. How to apply SBI in **Connectomics**

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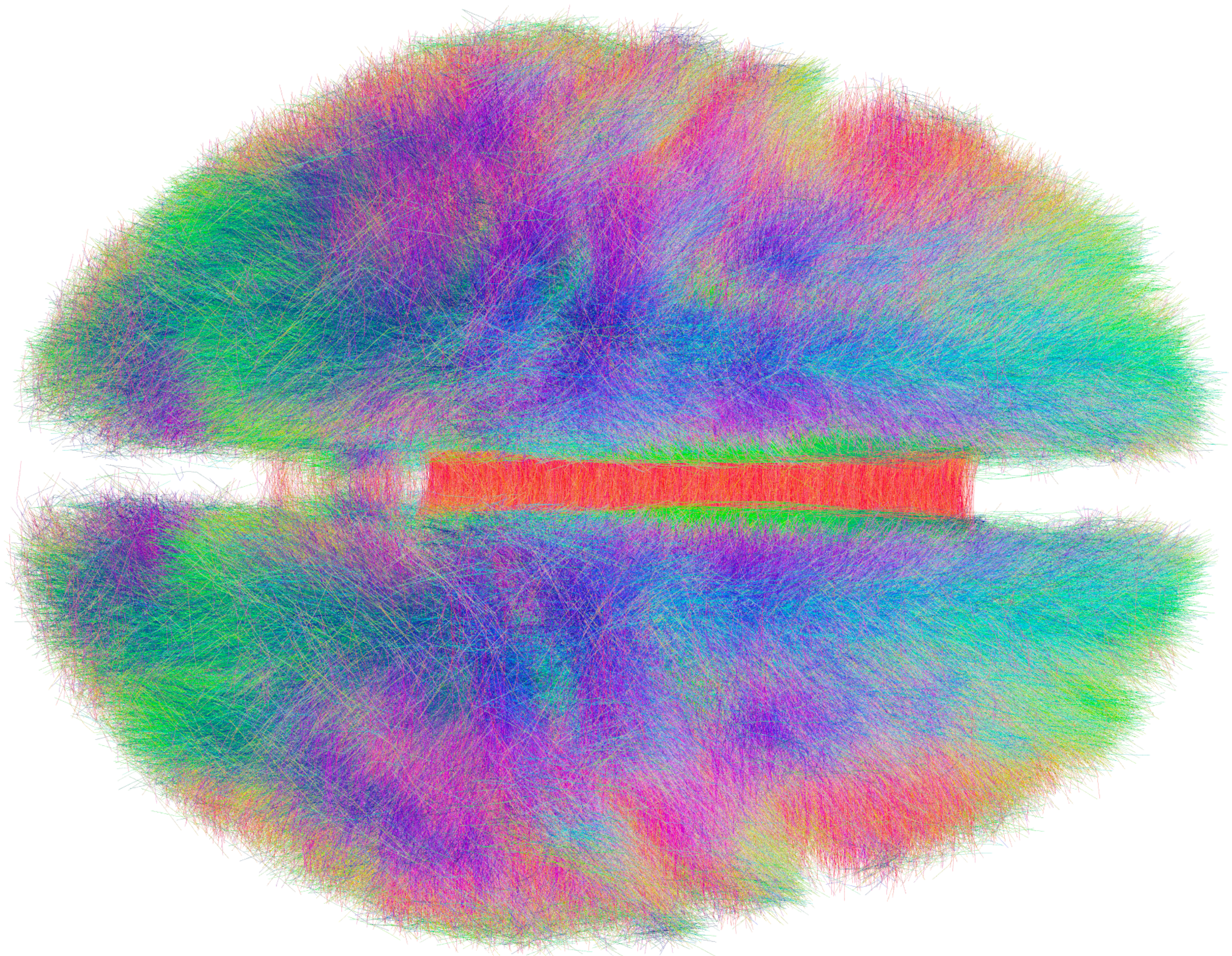
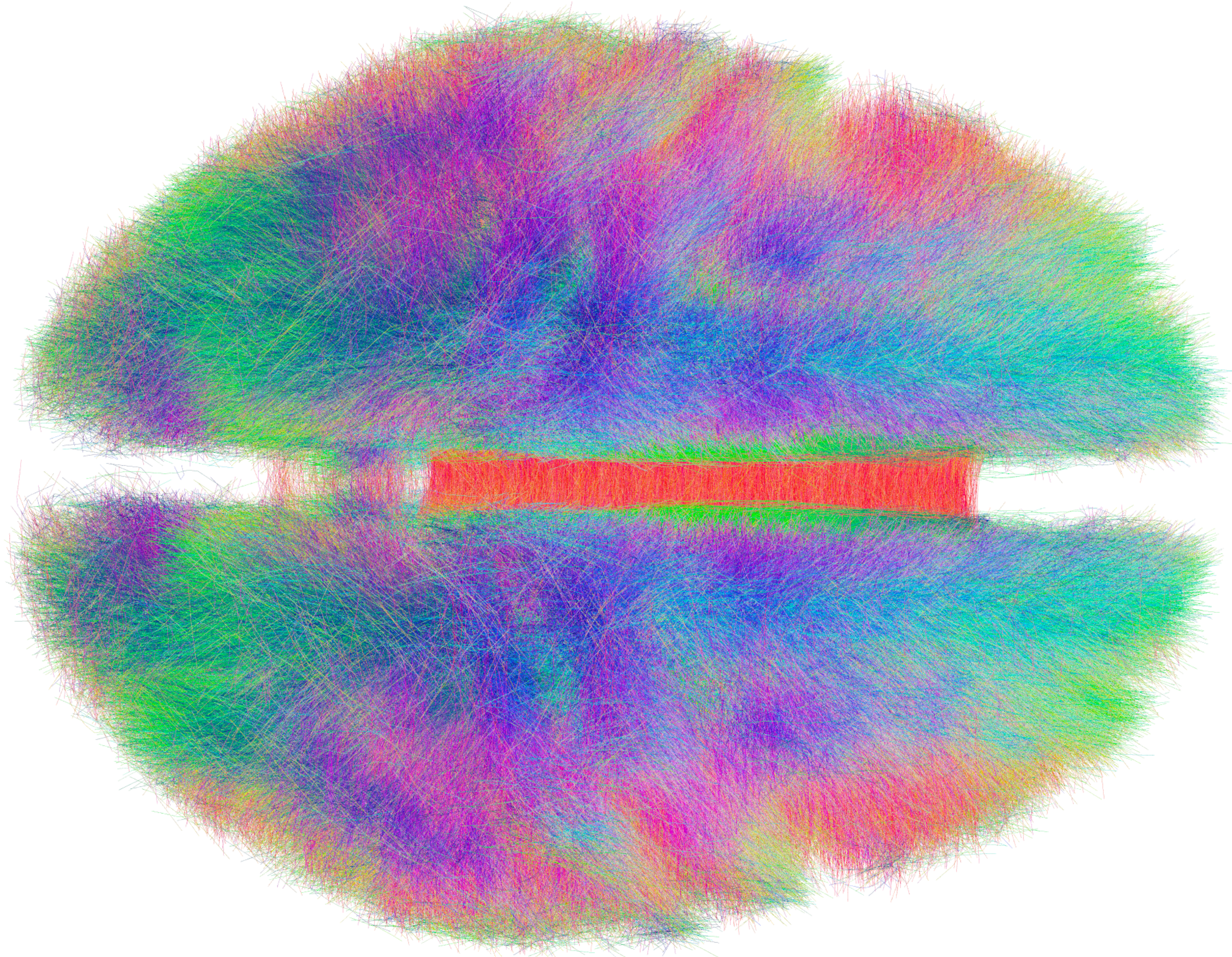
Connectomics:
unraveling the connectivity of the brain



macroscale connectomics

Wikipedia; Google / Lichtman lab; Winding et al. 2023

Connectomics: unraveling the connectivity of the brain



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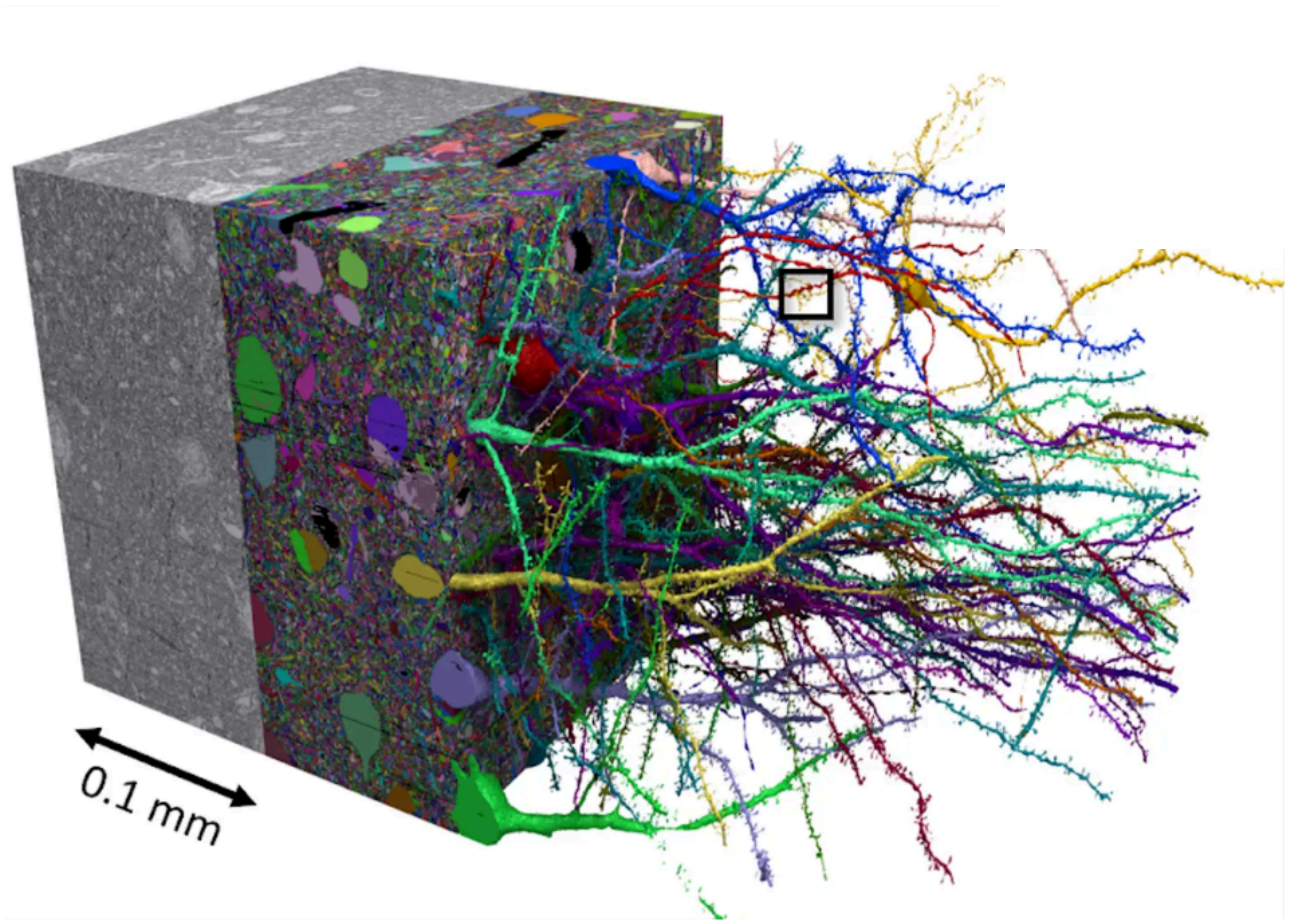

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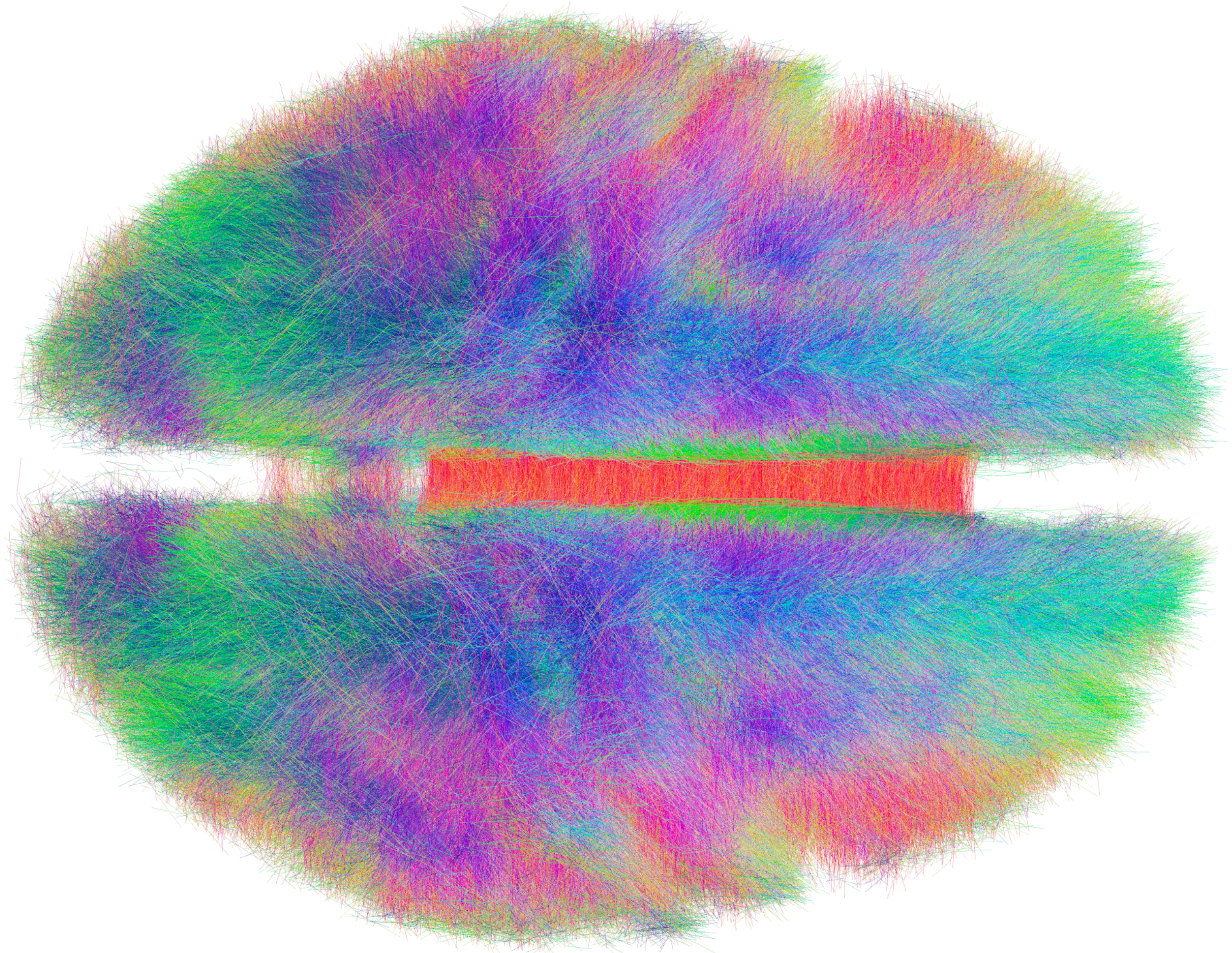

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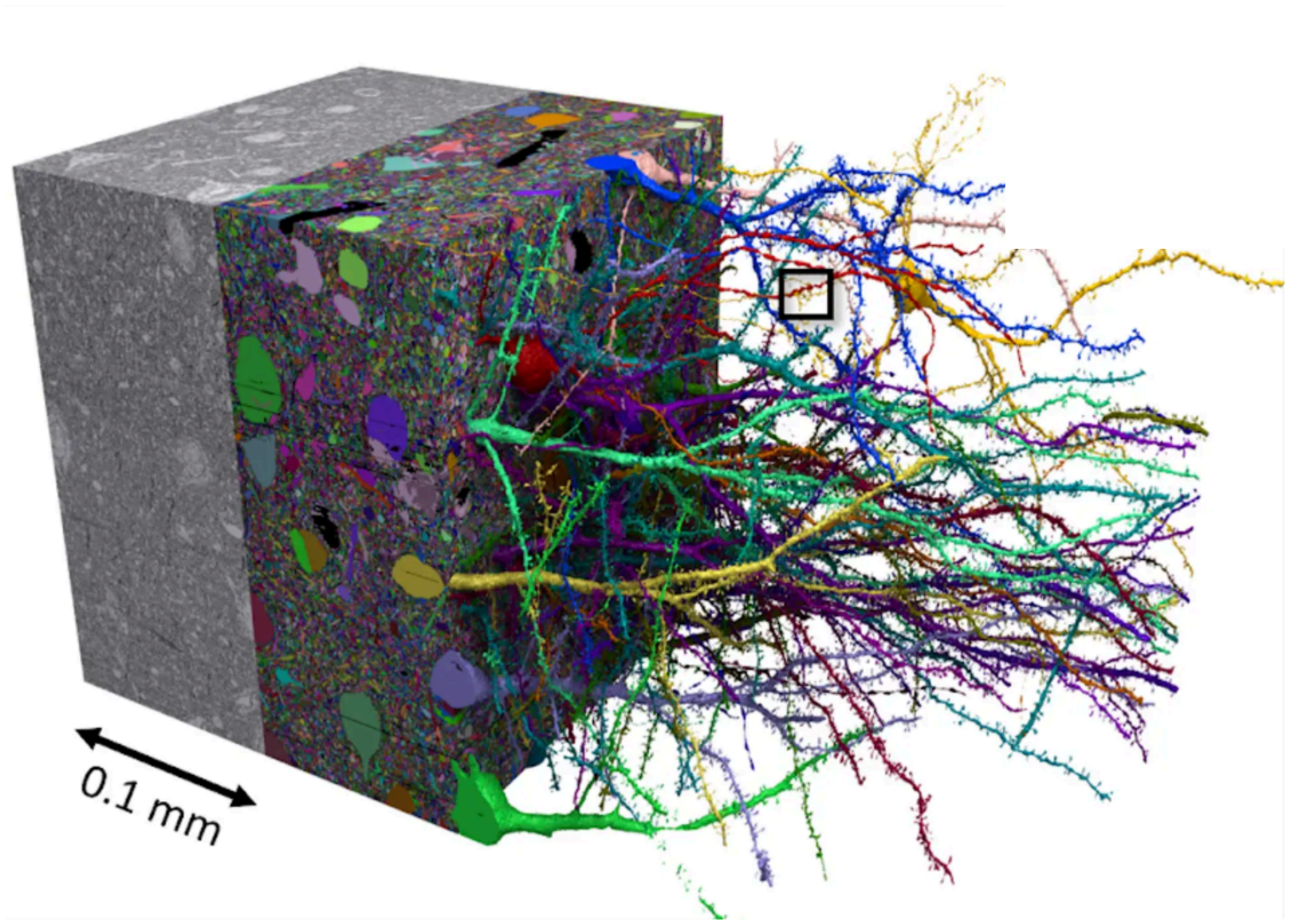

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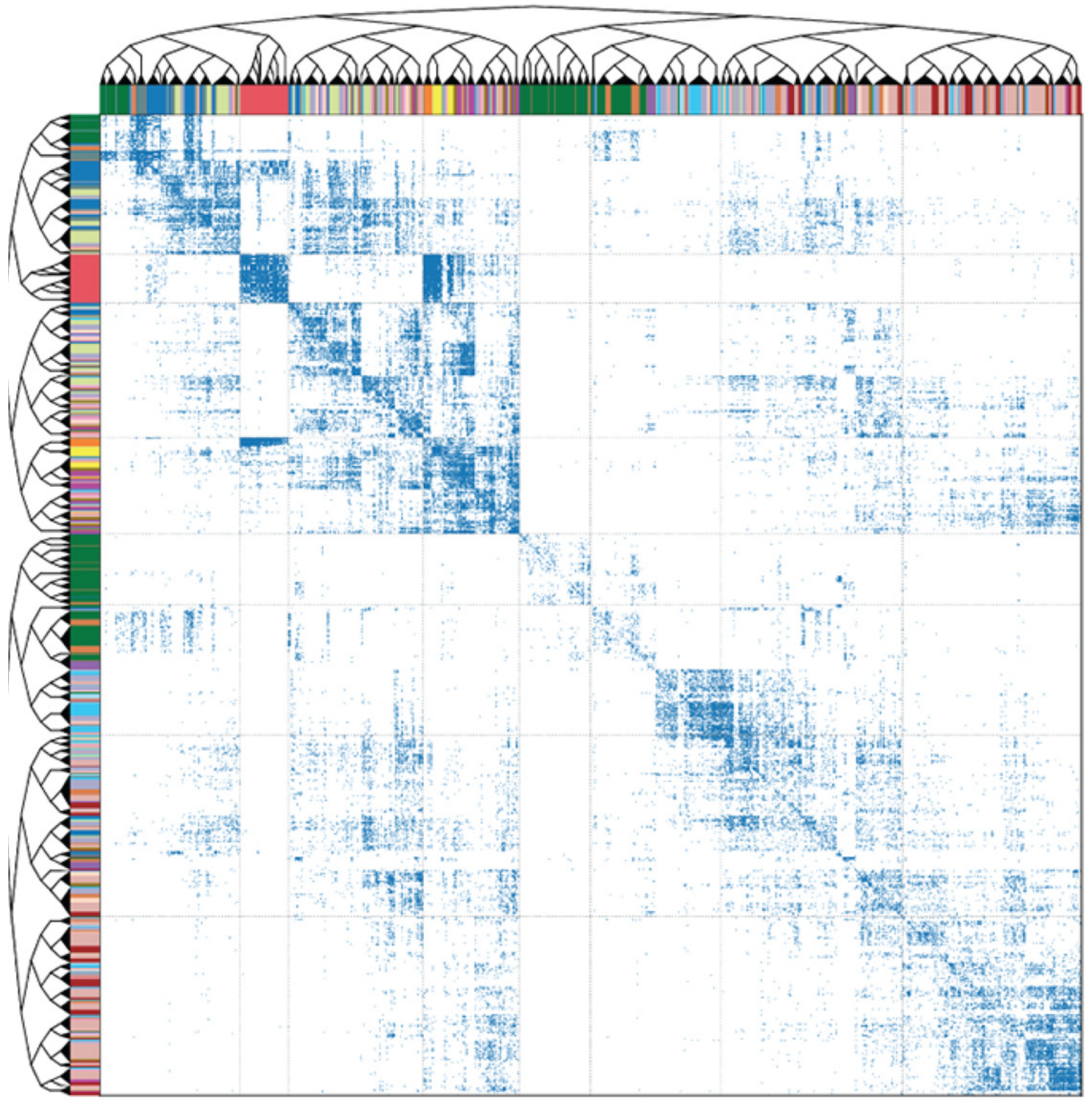

connectivity matrix

Wikipedia; Google / Lichtman lab; Winding et al. 2023

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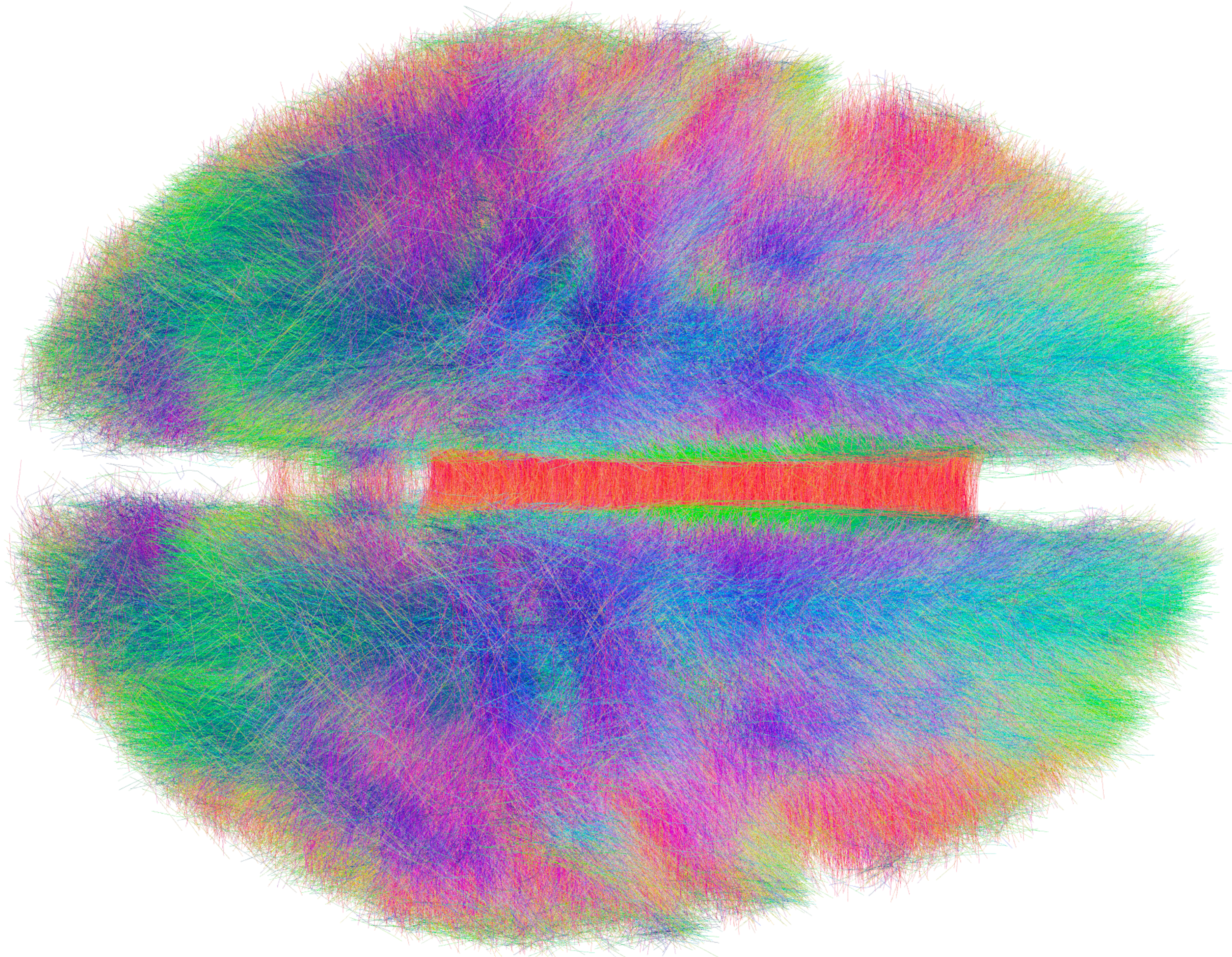

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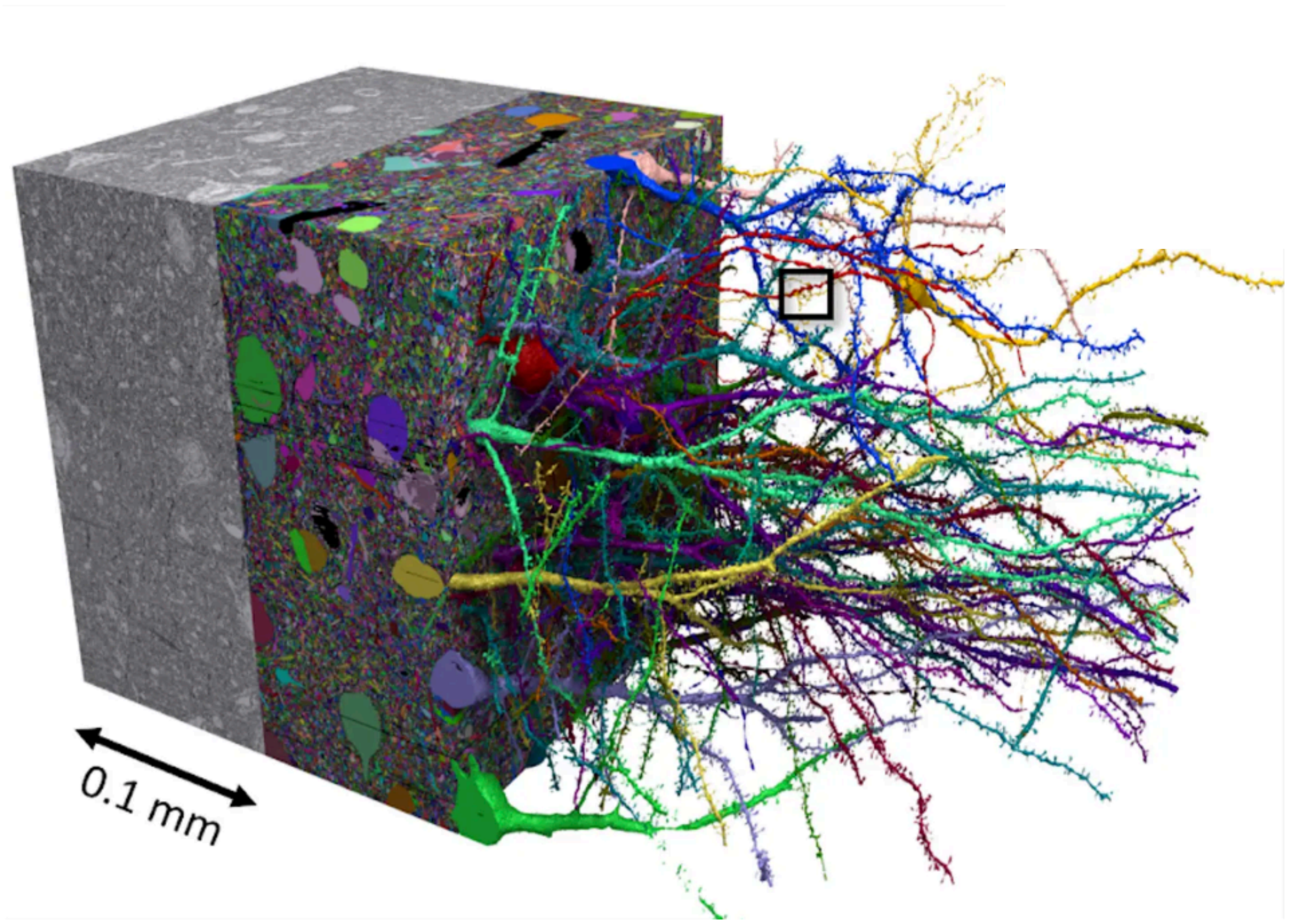

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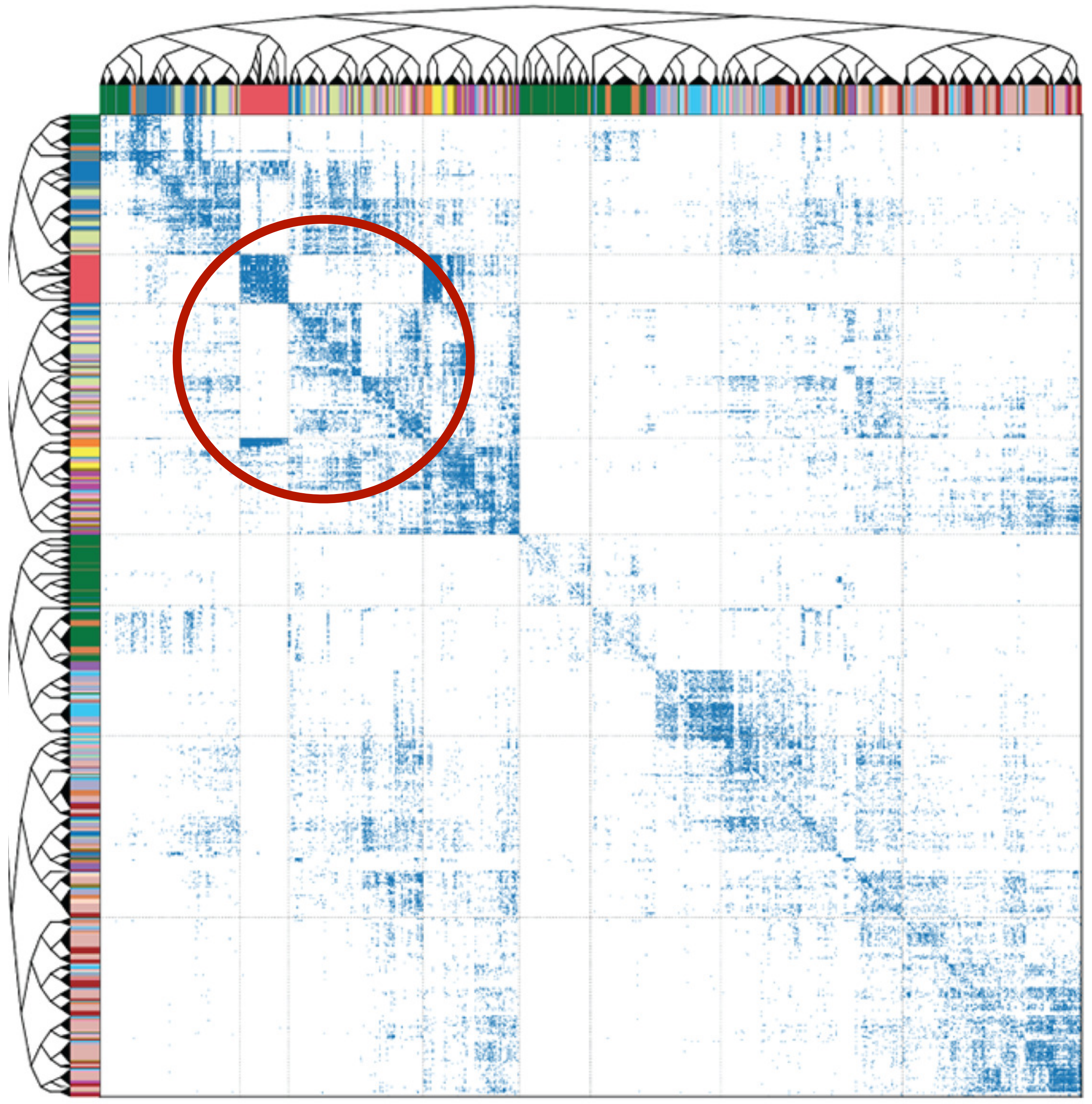

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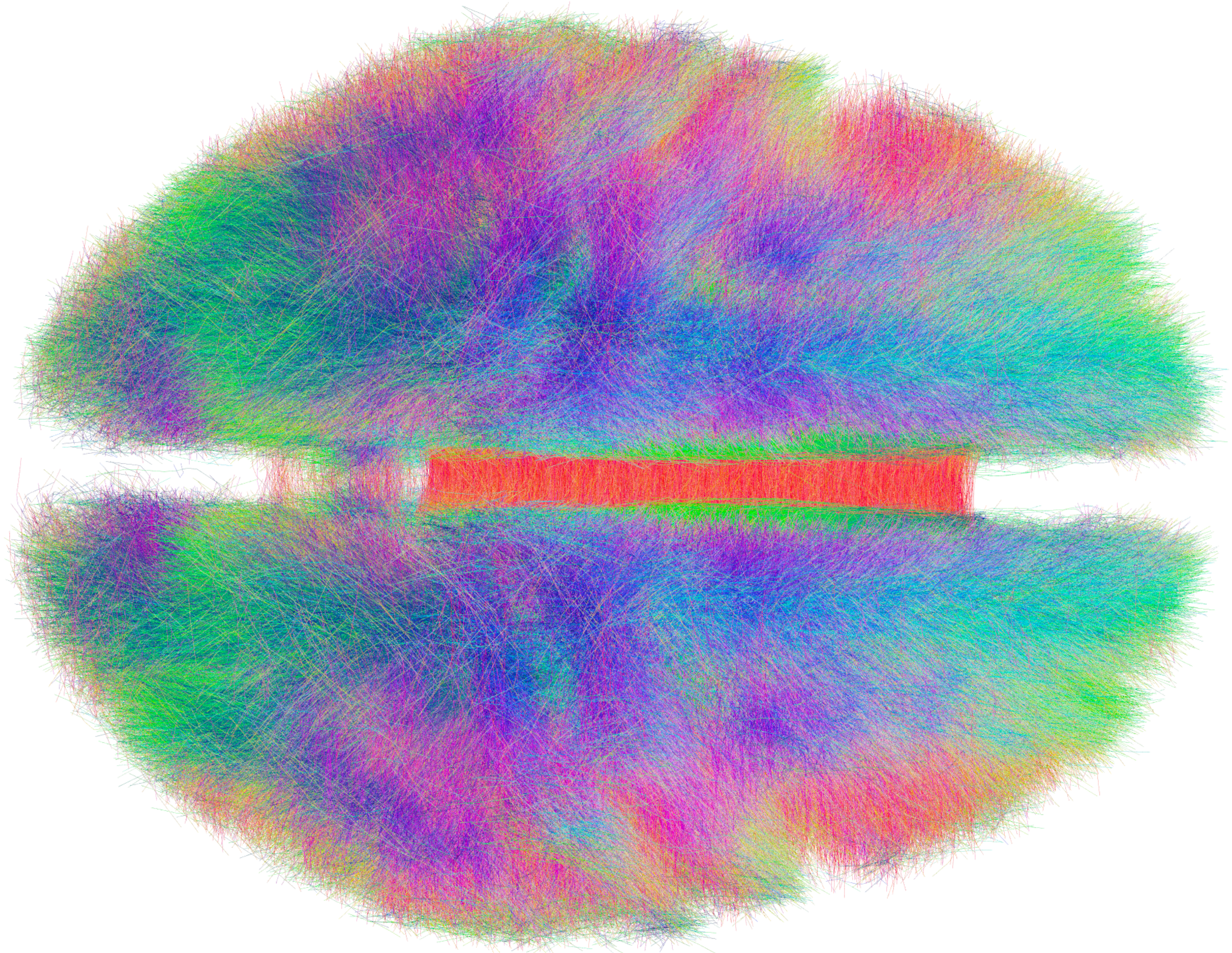
Connectomics: unraveling the connectivity of the brain



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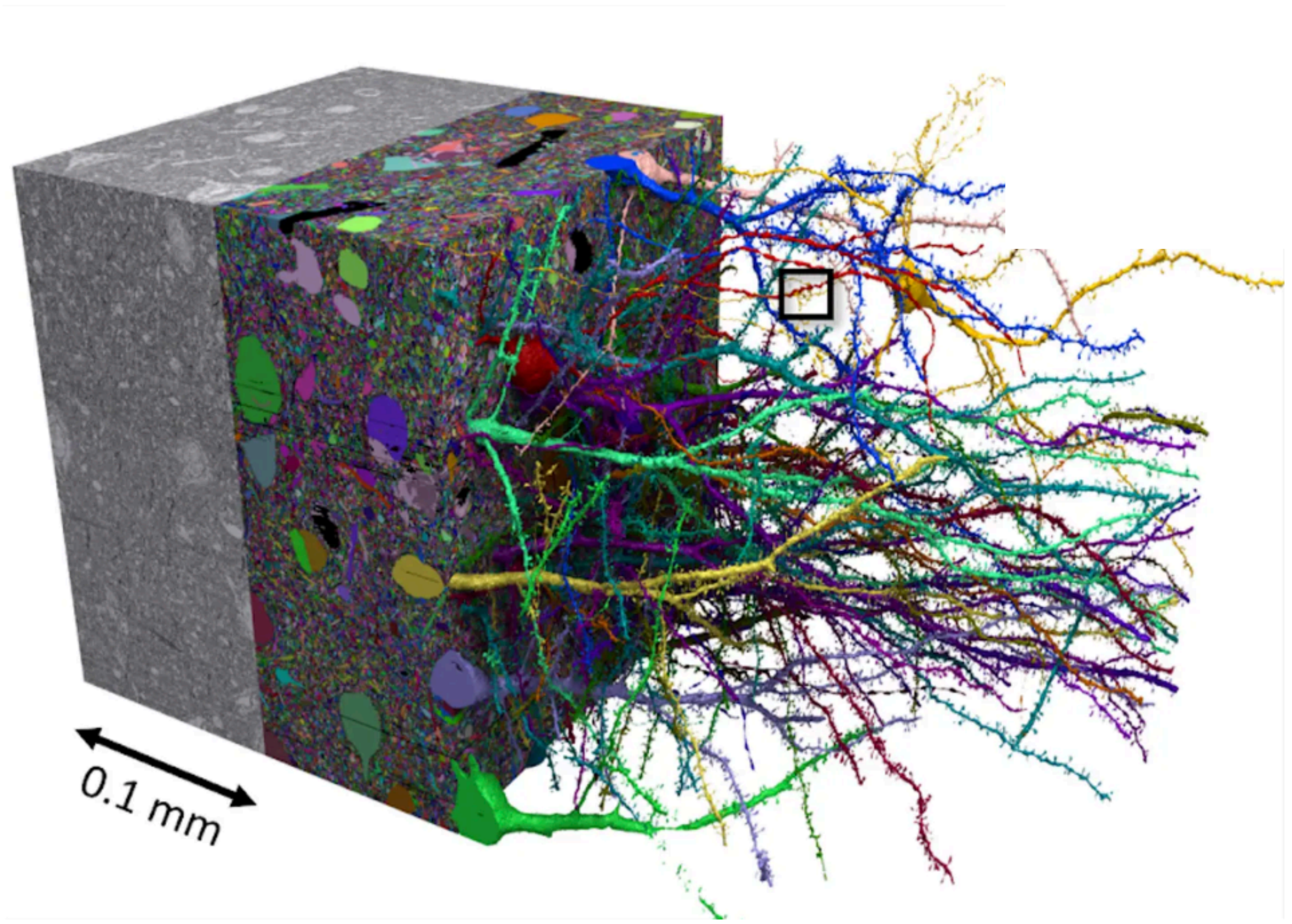

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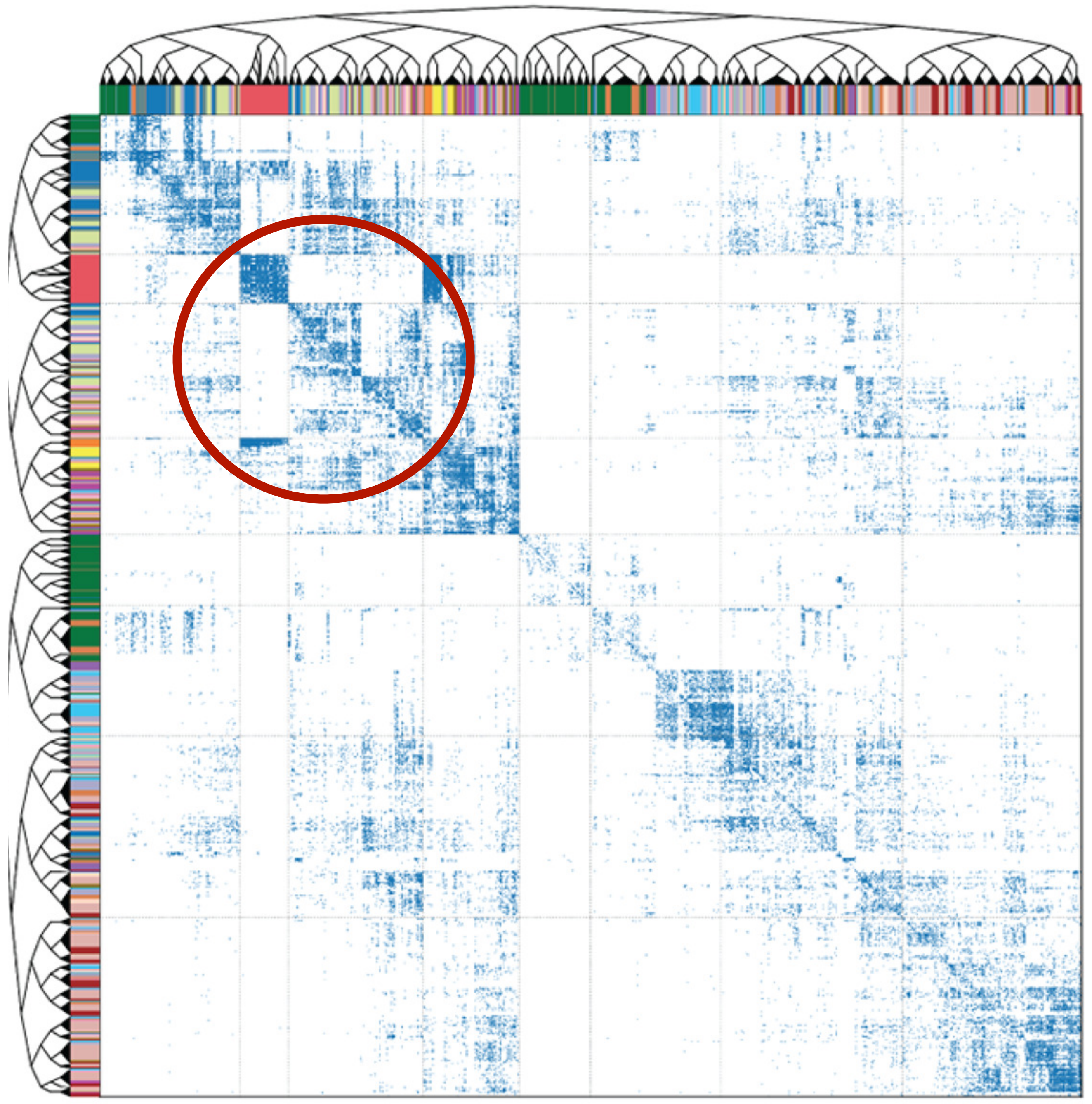
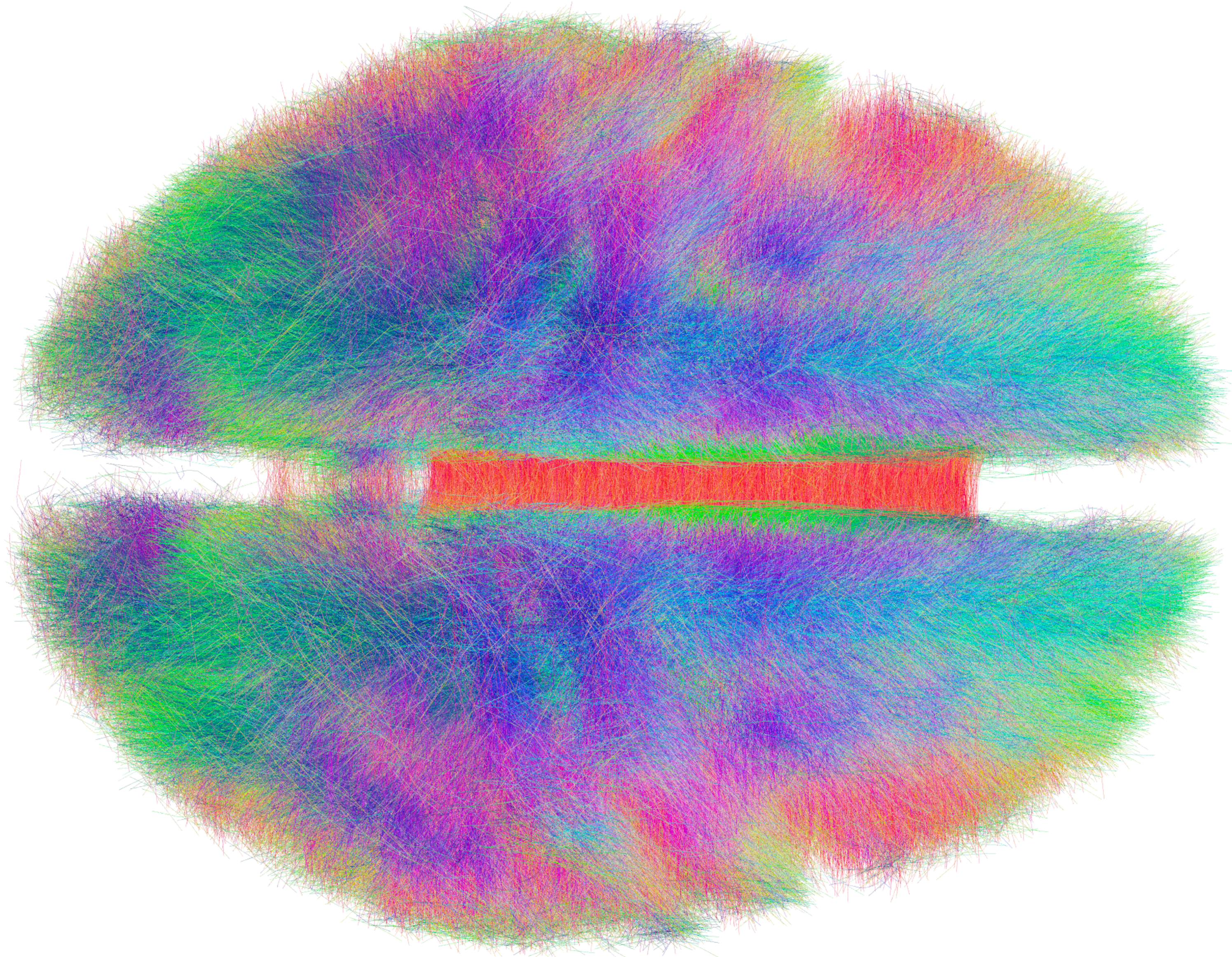


connectivity matrix

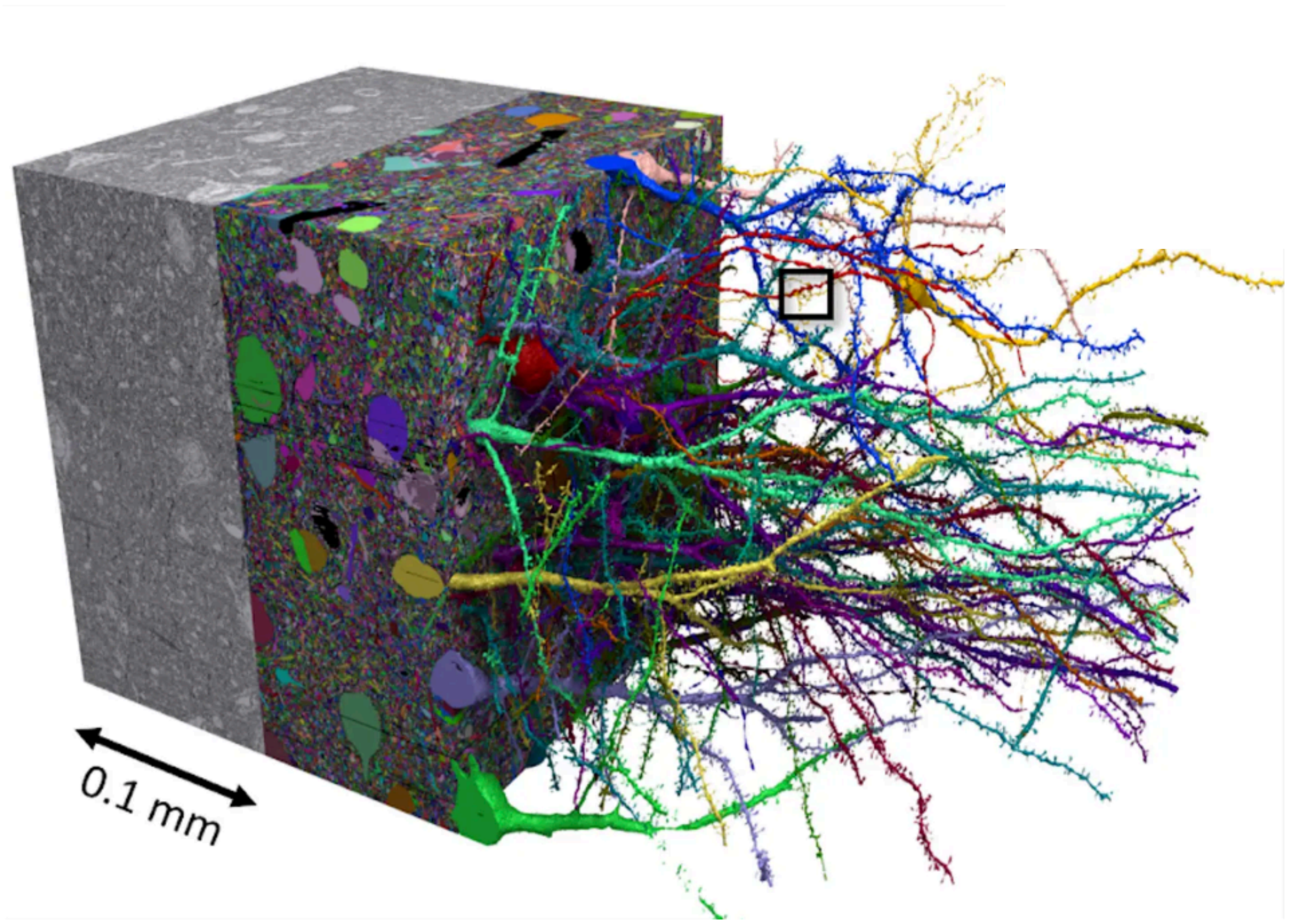
- How do connectivity patterns emerge?

Wikipedia; Google / Lichtman lab; Winding et al. 2023

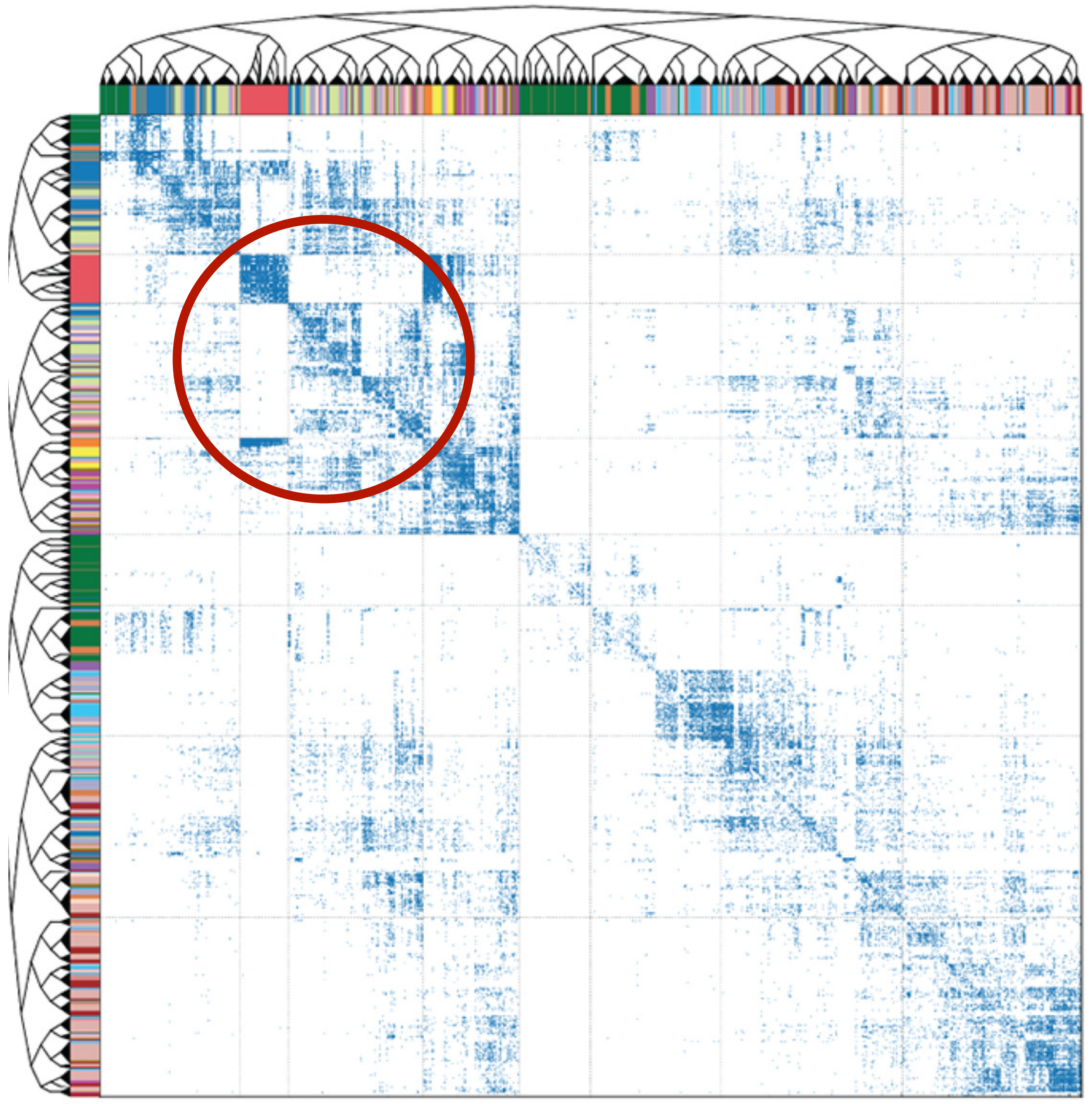
Connectomics: unraveling the connectivity of the brain



macroscale connectomics



microscale connectomics

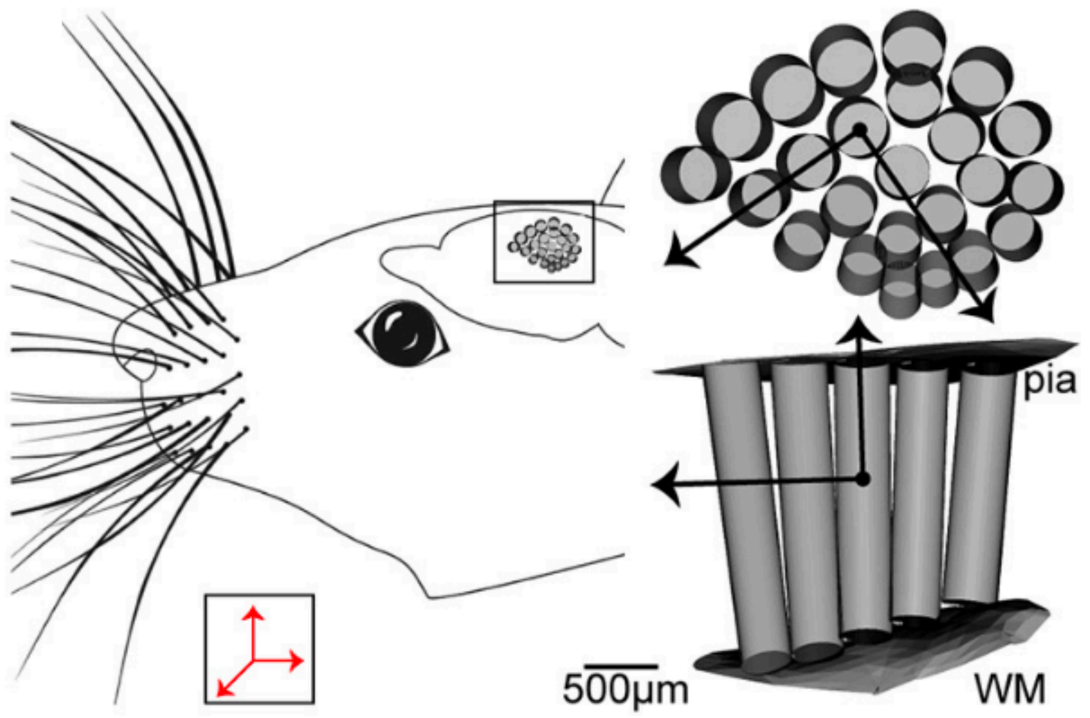


connectivity matrix

- How do connectivity patterns emerge?
- Are there general **wiring rules** that determine the connectivity patterns?

Wikipedia; Google / Lichtman lab; Winding et al. 2023

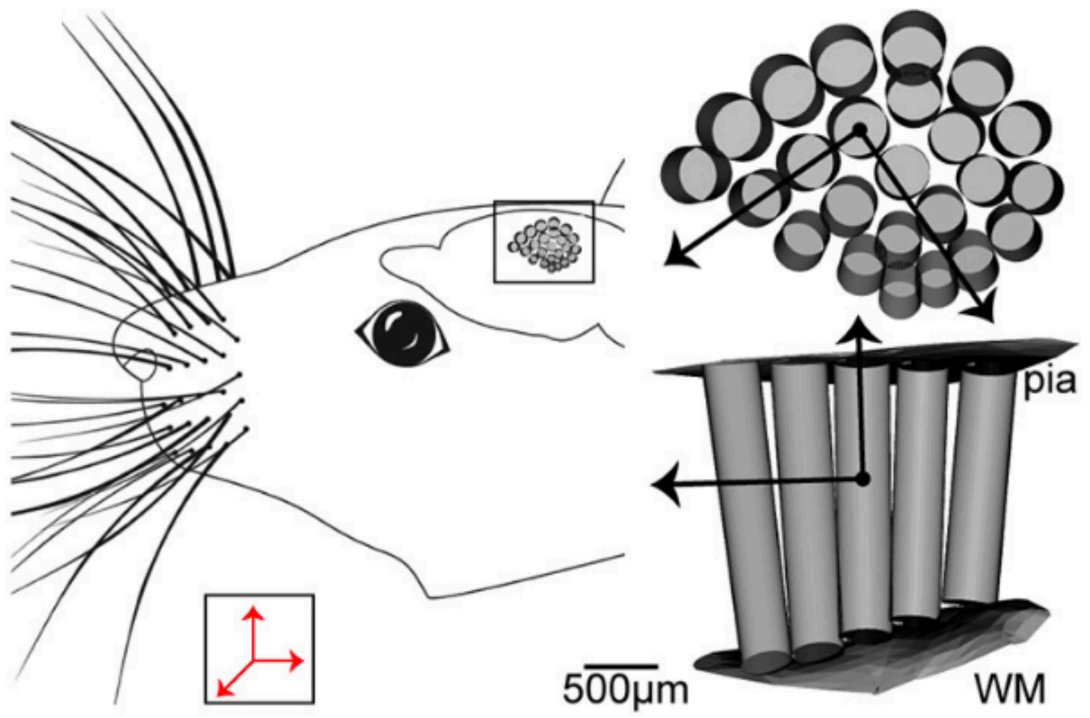
A computer model of the rat barrel cortex



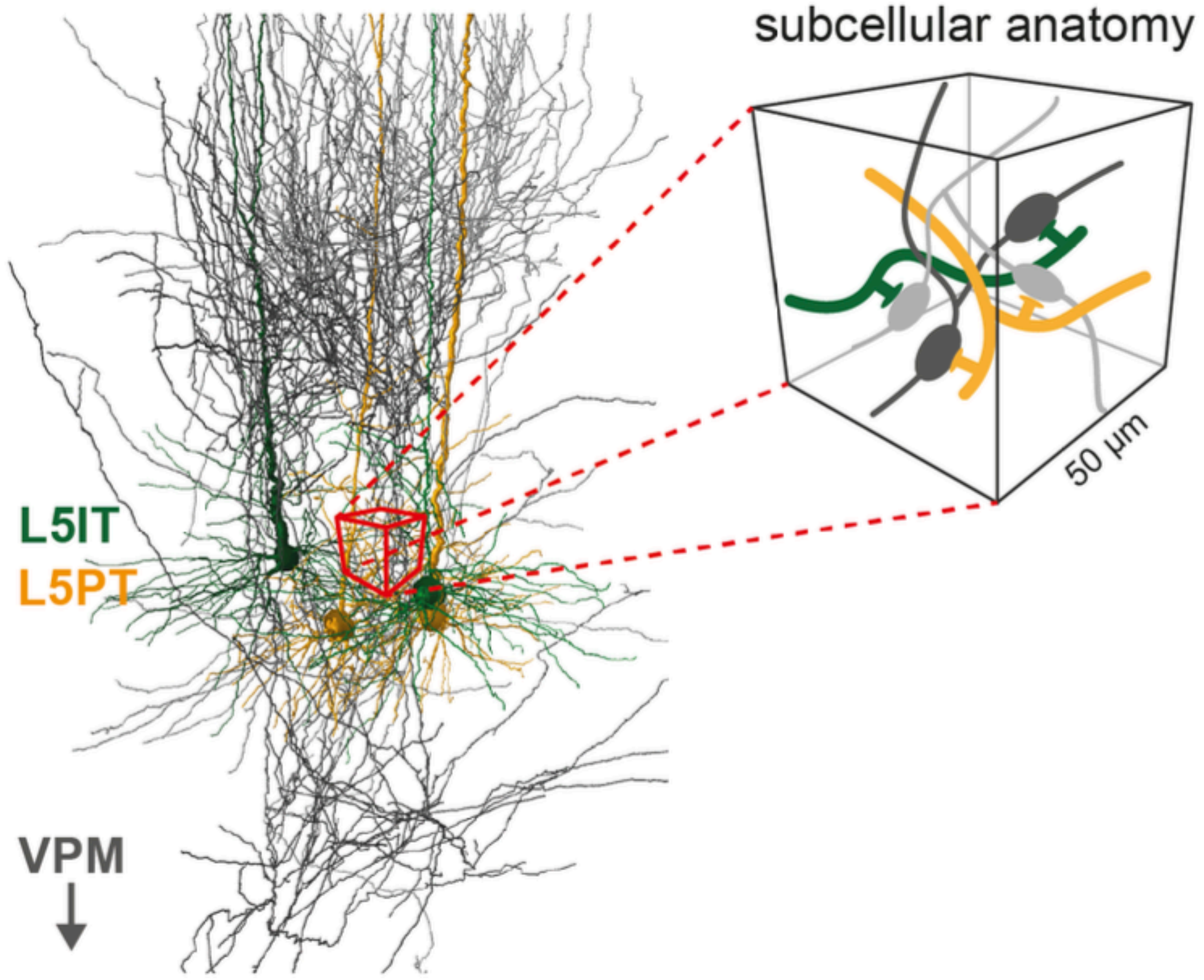
rat barrel cortex

Egger et al. 2014; Udvary et al. 2022

A computer model of the rat barrel cortex



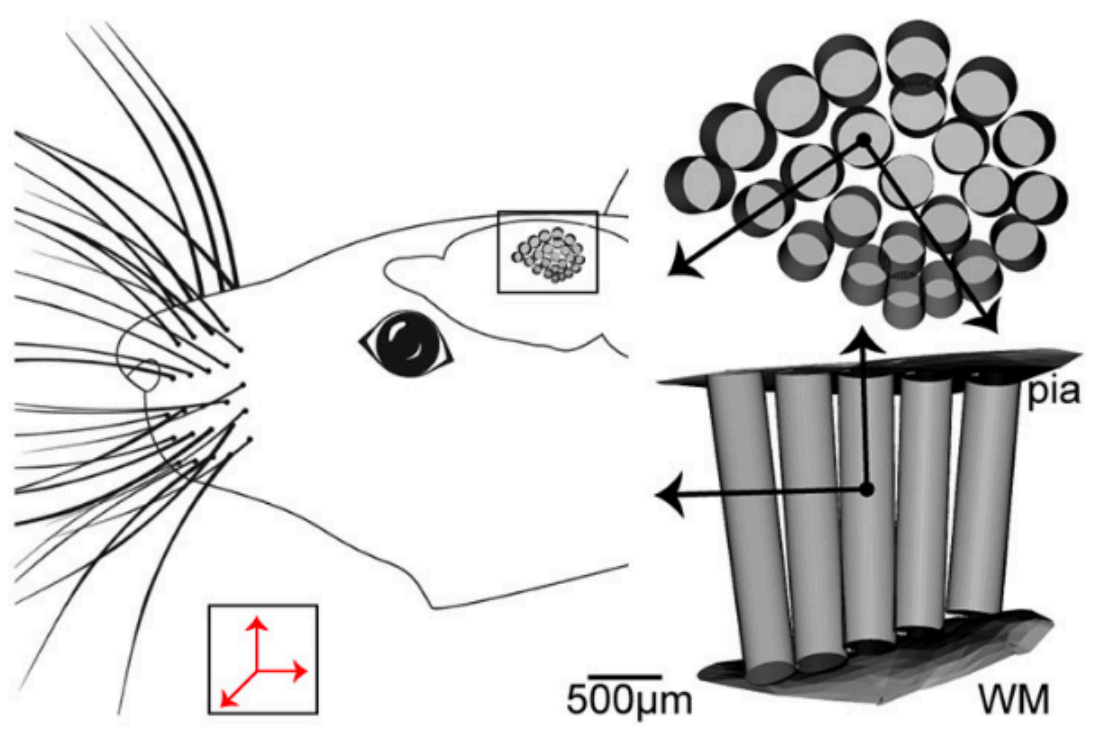
rat barrel cortex



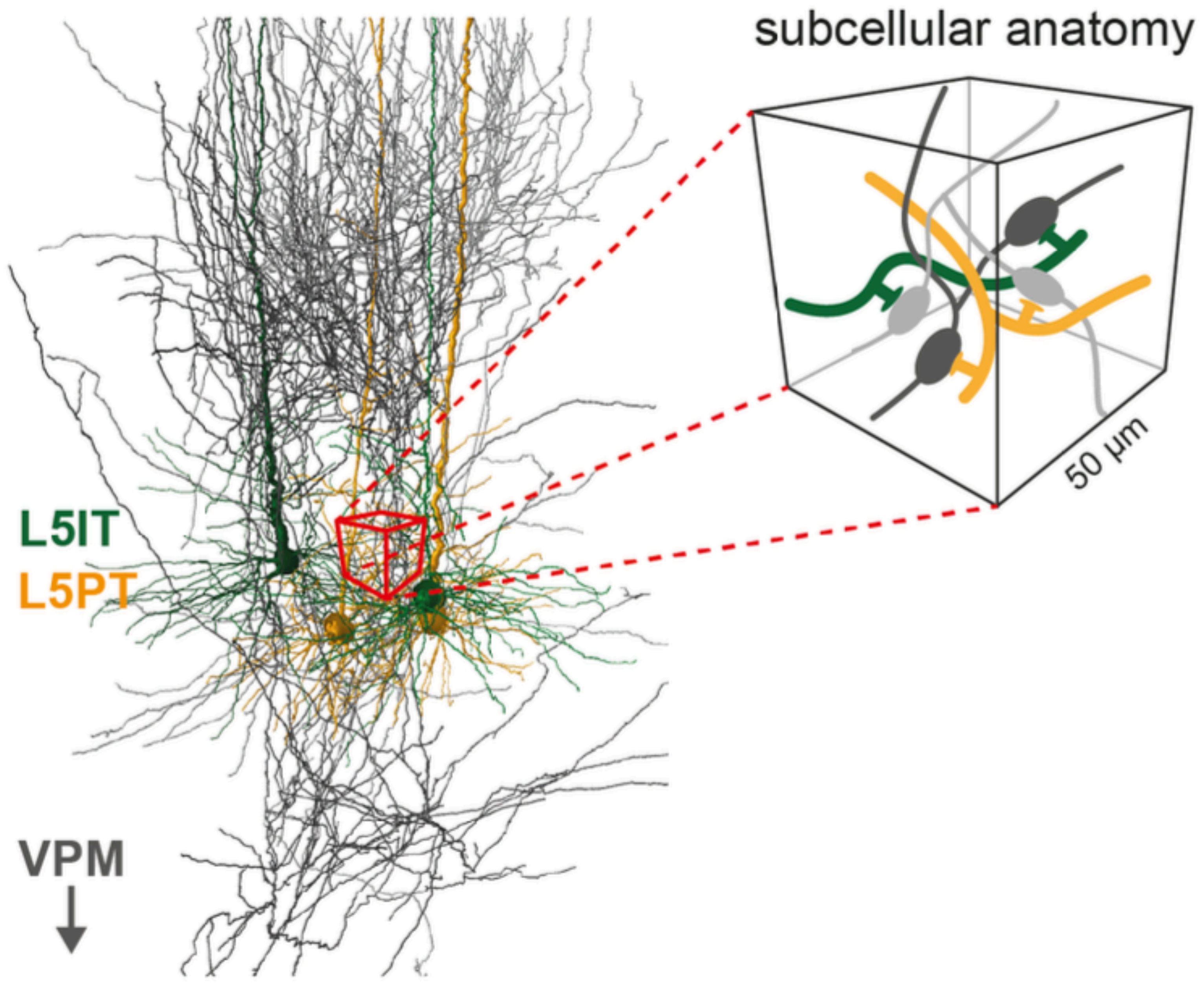
reconstruction of neurons

Egger et al. 2014; Udvary et al. 2022

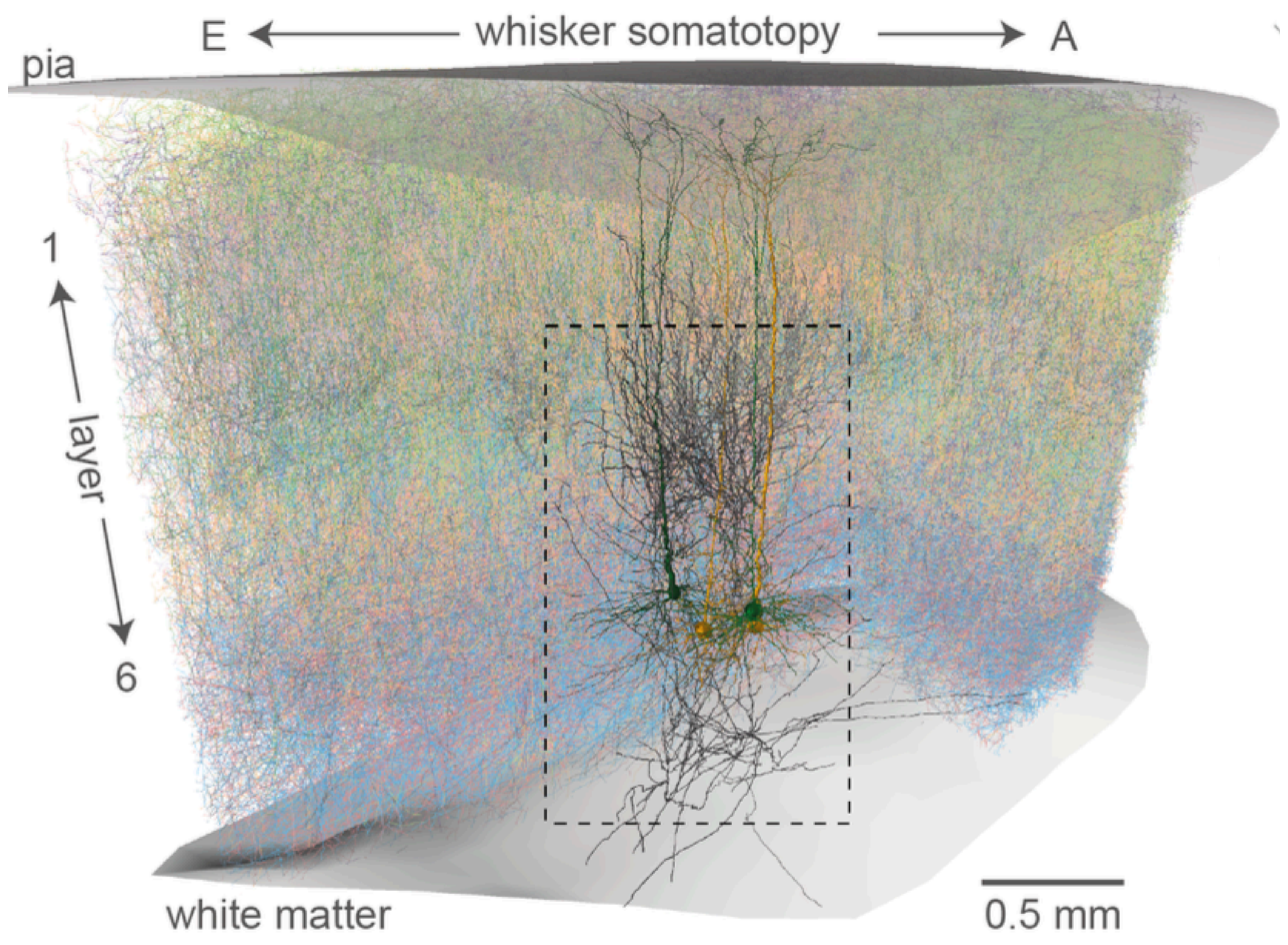
A computer model of the rat barrel cortex



rat barrel cortex



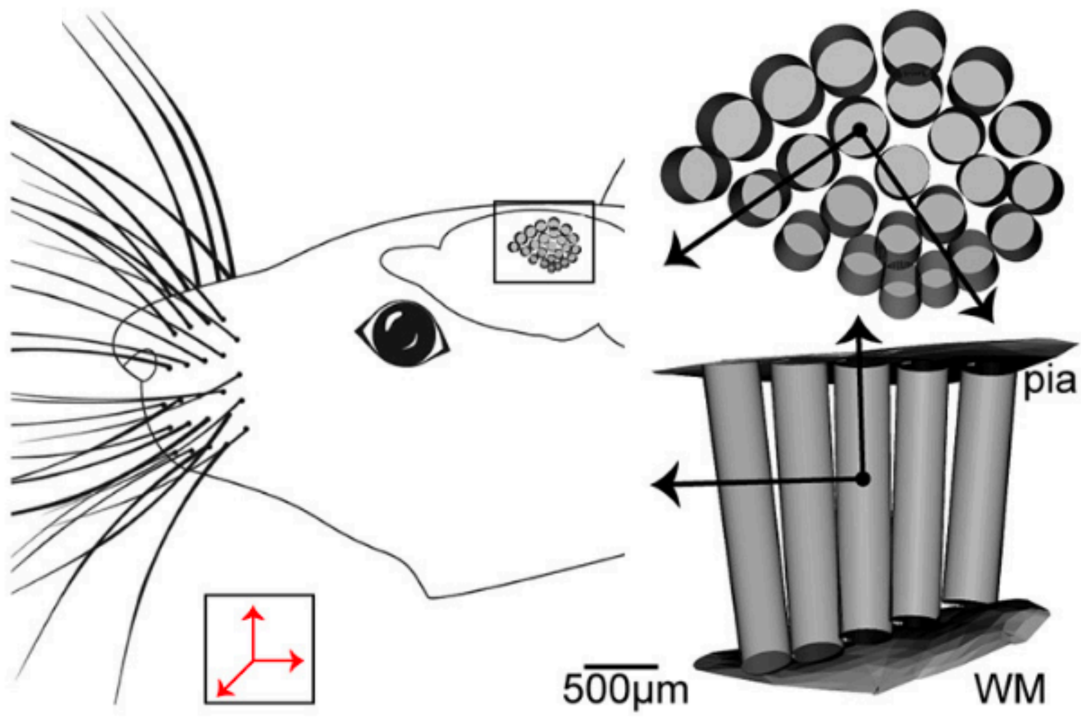
reconstruction of neurons



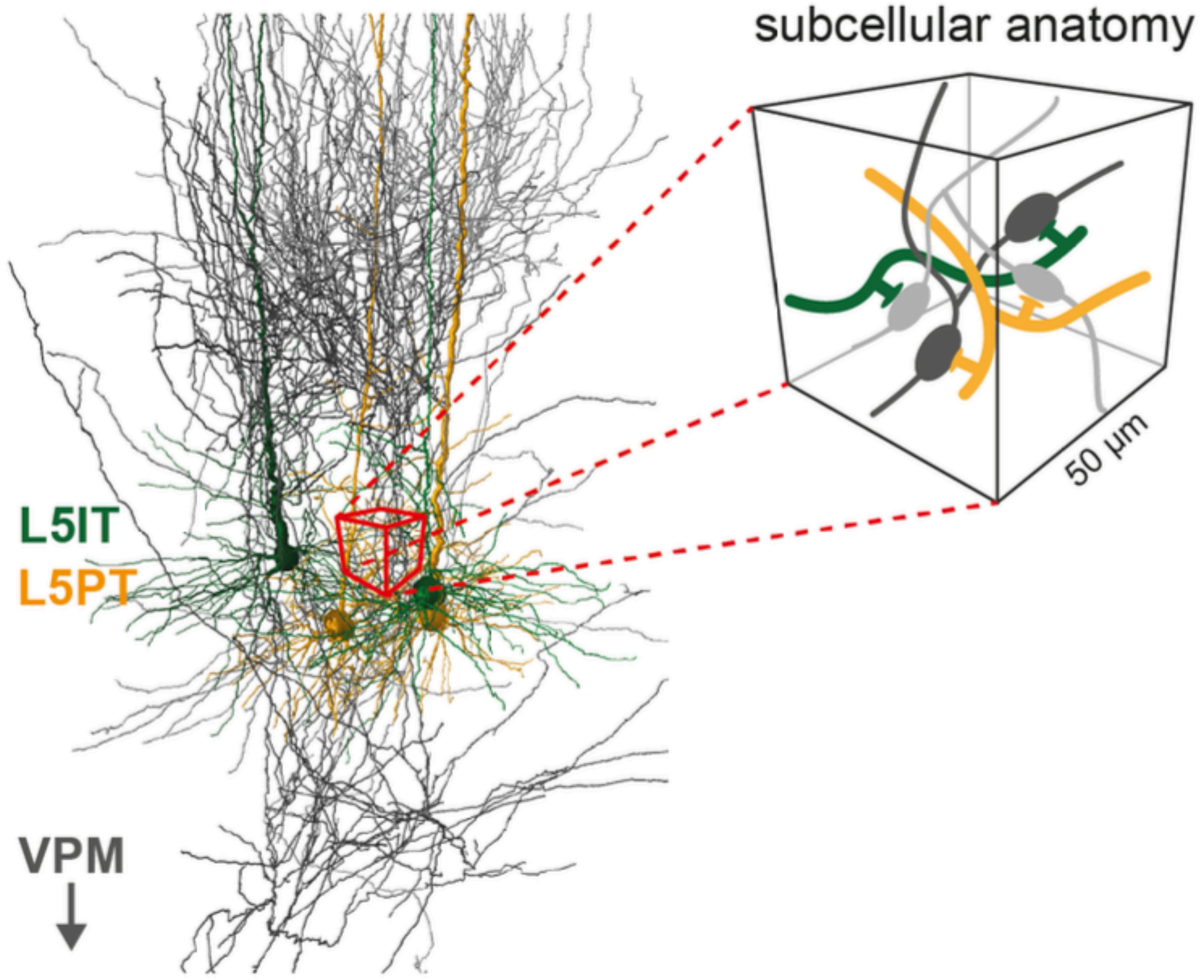
3D model of the barrel cortex

Egger et al. 2014; Udvary et al. 2022

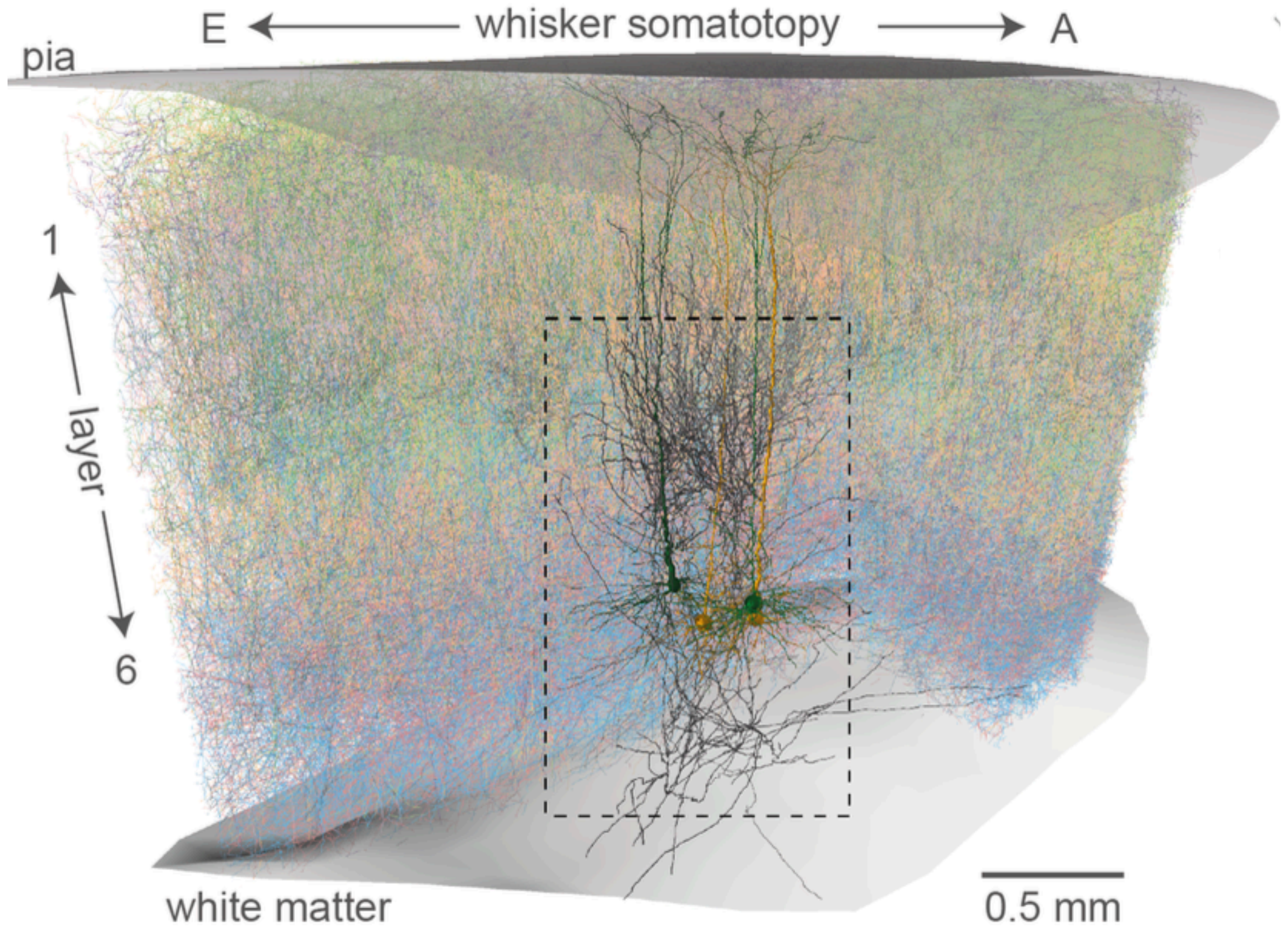
A computer model of the rat barrel cortex



rat barrel cortex



reconstruction of neurons

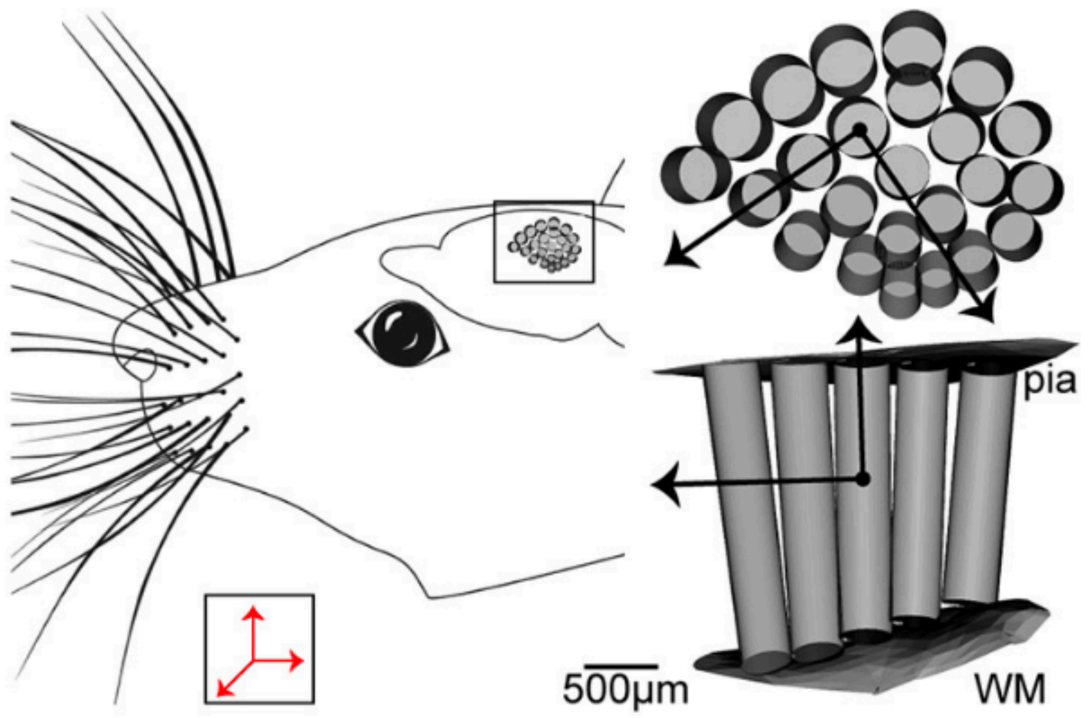


3D model of the barrel cortex

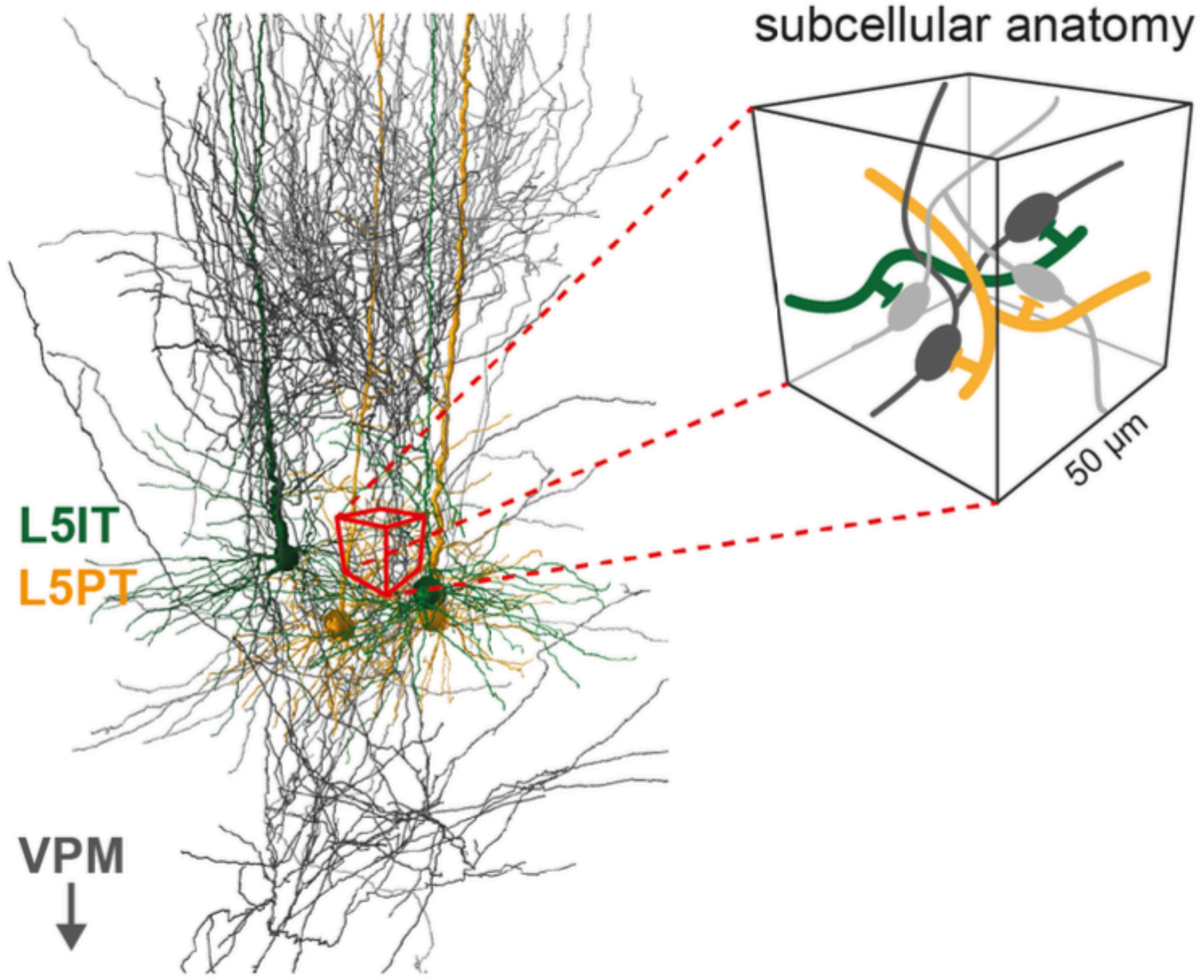
- Model contains only structure, **no connections**

Egger et al. 2014; Udvary et al. 2022

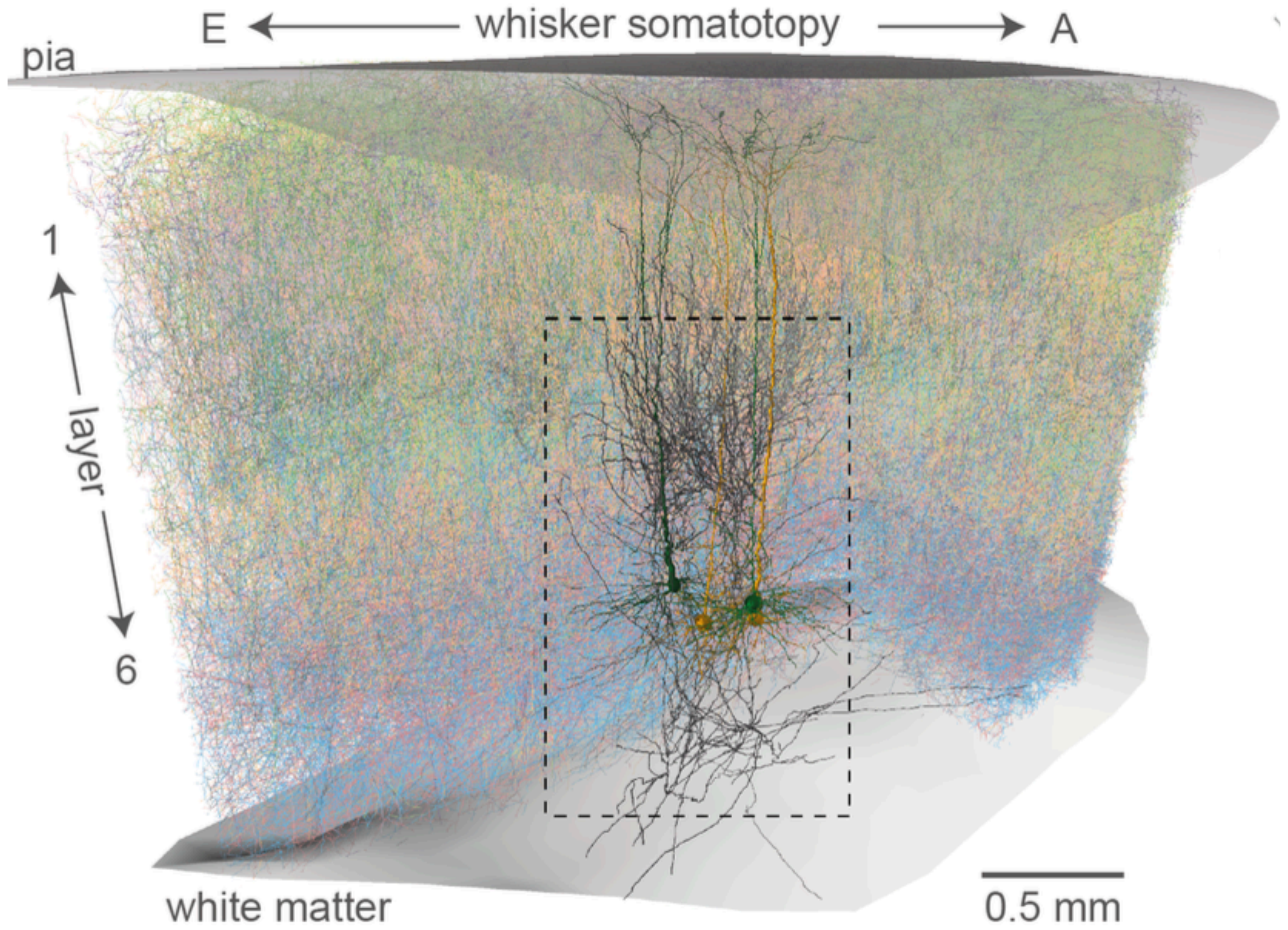
A computer model of the rat barrel cortex



rat barrel cortex



reconstruction of neurons

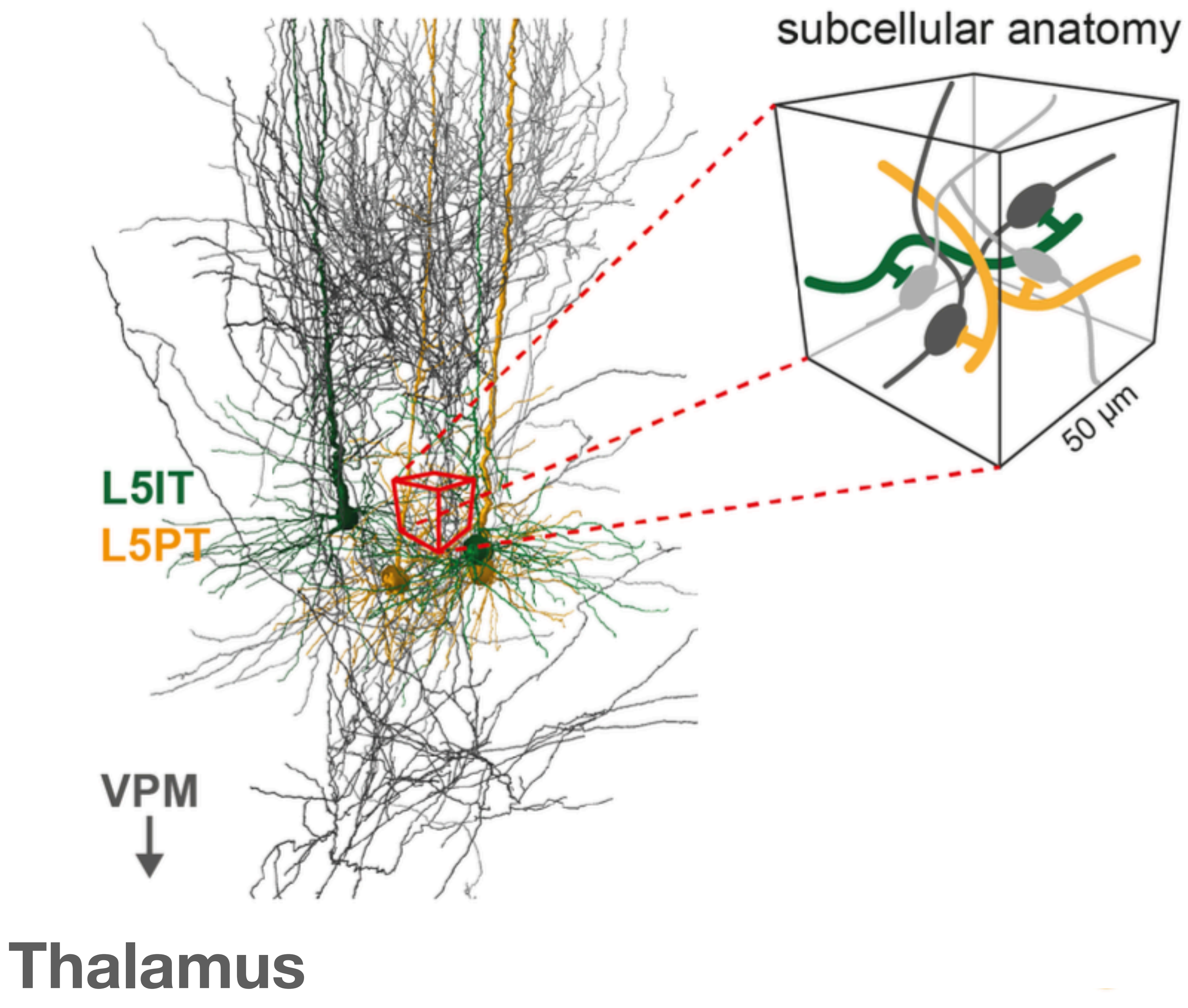


3D model of the barrel cortex

- Model contains only structure, **no connections**
- Provides a **testing ground for wiring rules**

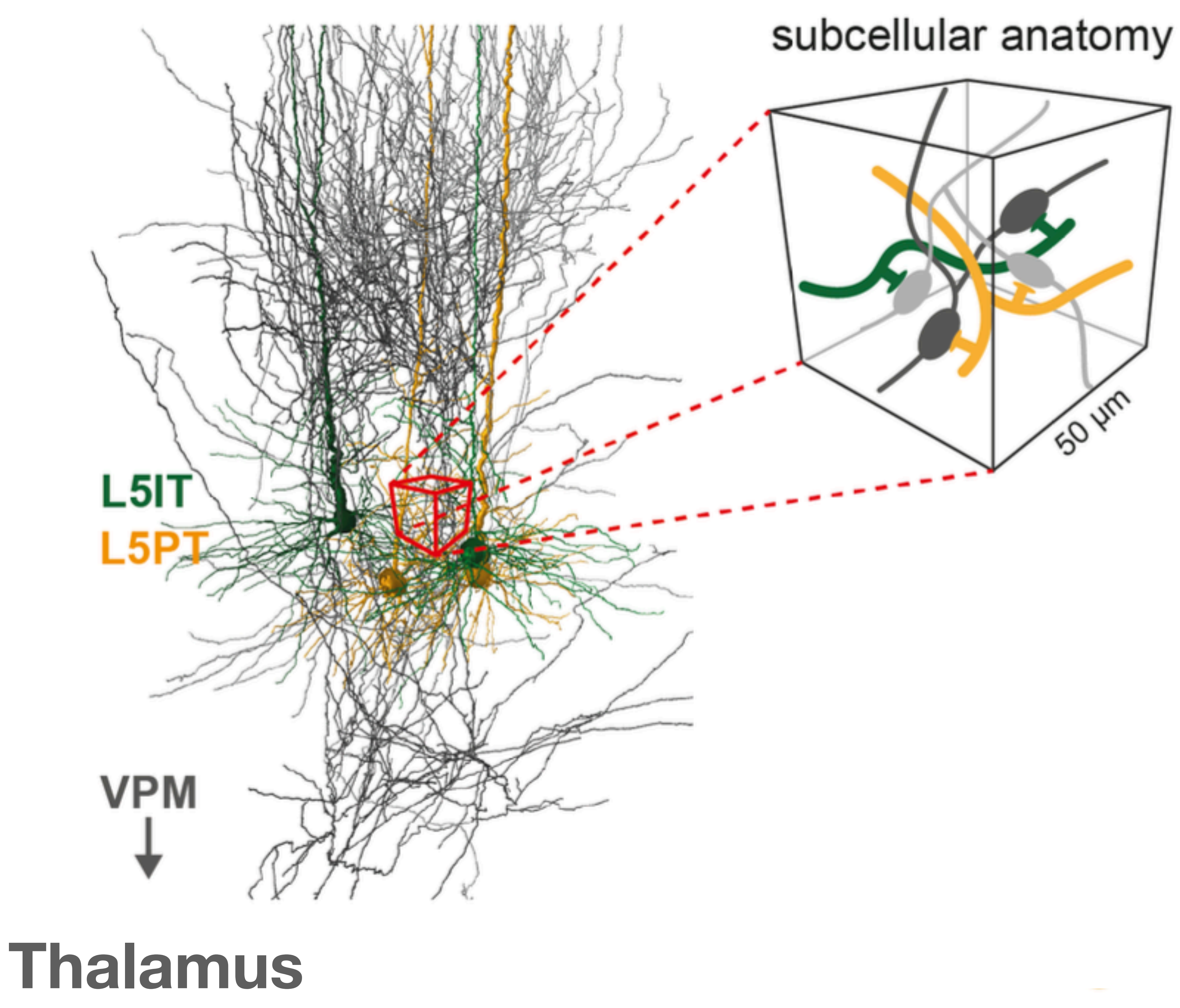
Egger et al. 2014; Udvary et al. 2022

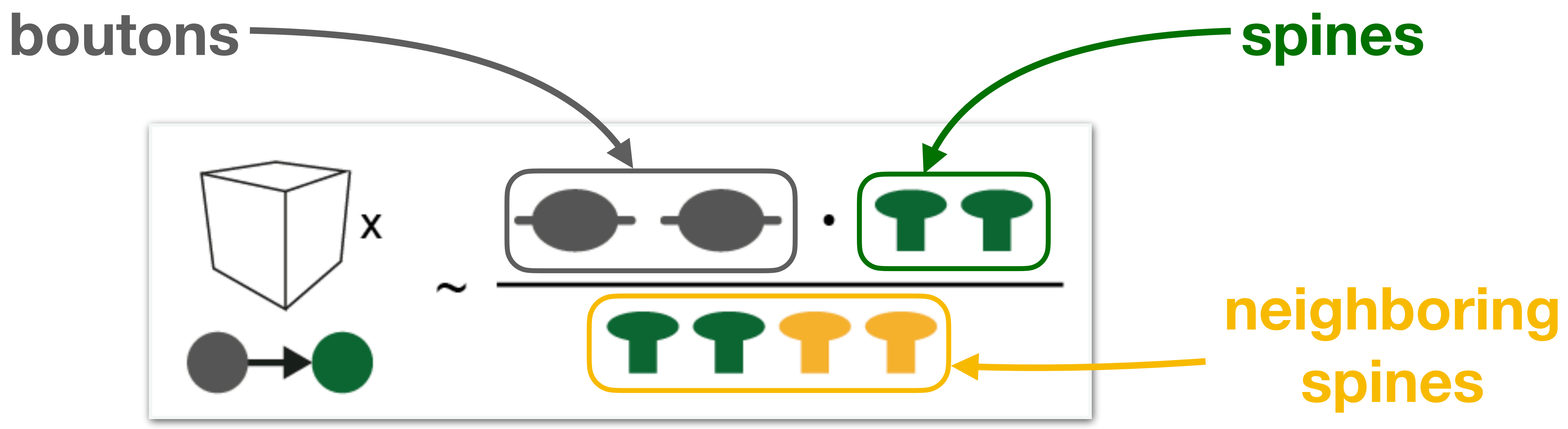
A structural wiring rule for the barrel cortex



Boelts et al. 2023; Udvary et al. 2022

A structural wiring rule for the barrel cortex

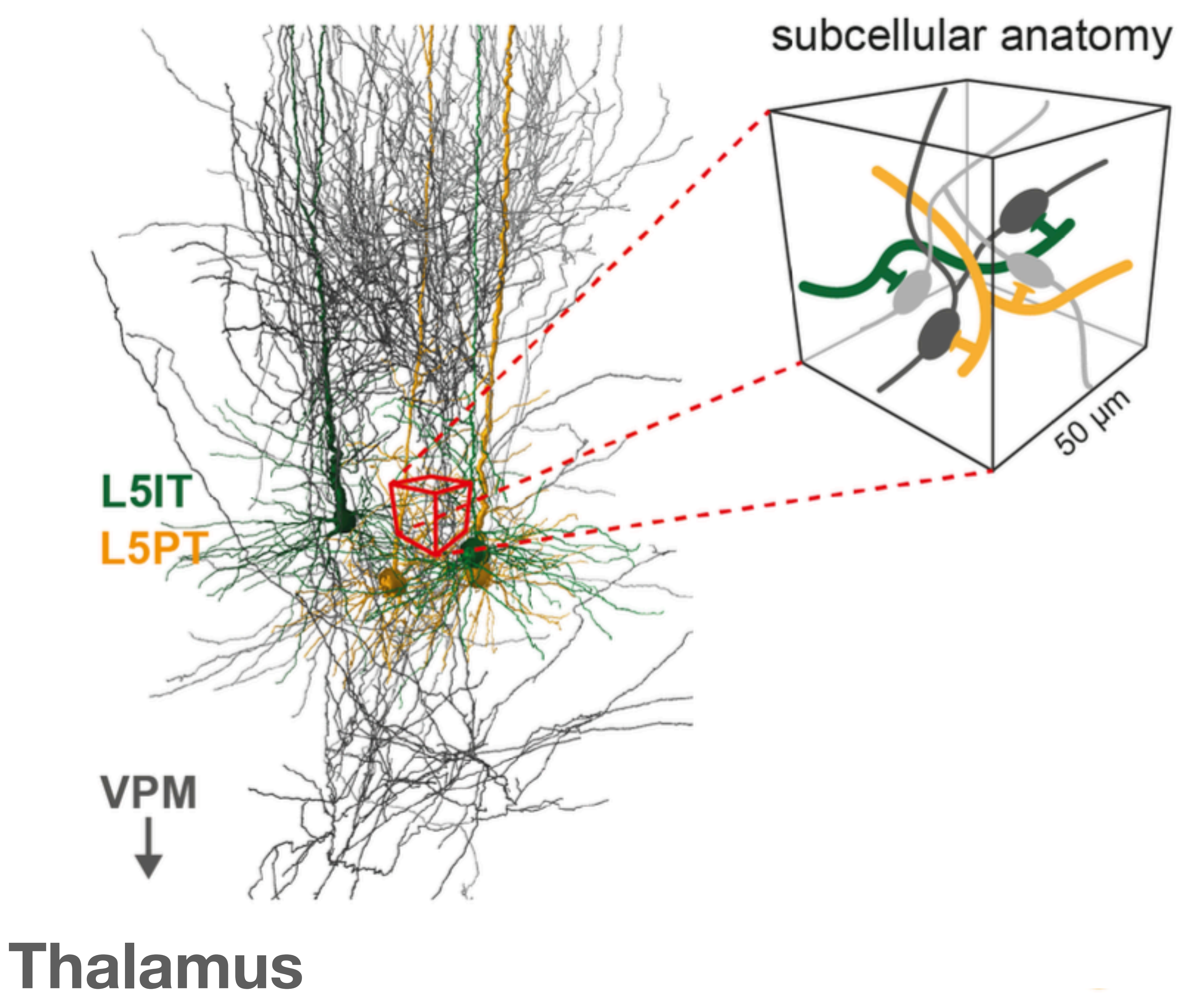


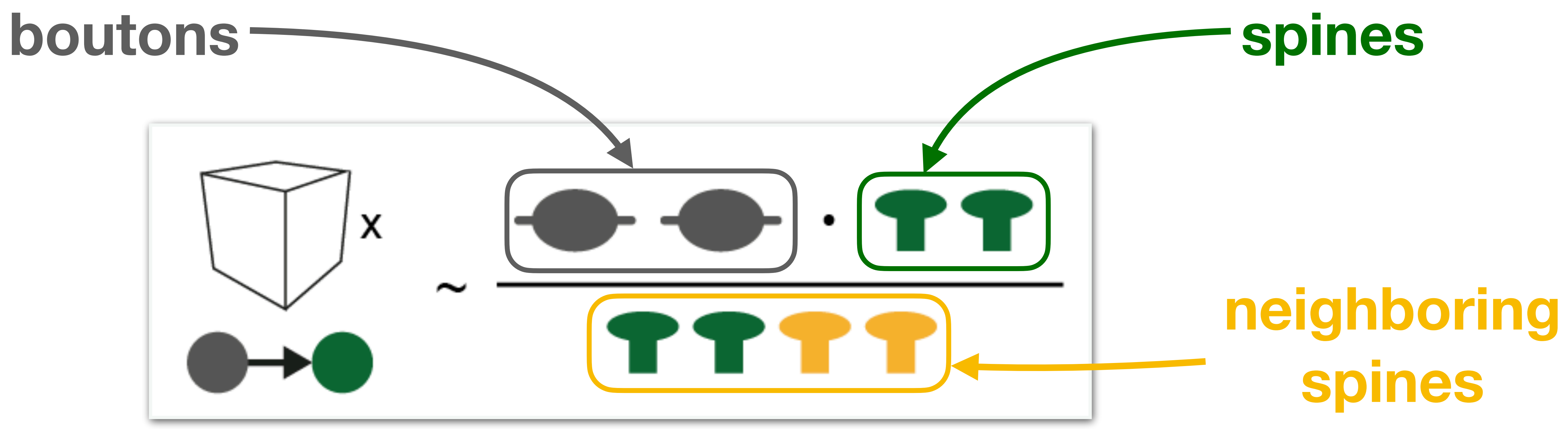


Dense Structural Overlap (DSO)

Boelts et al. 2023; Udvary et al. 2022

A structural wiring rule for the barrel cortex



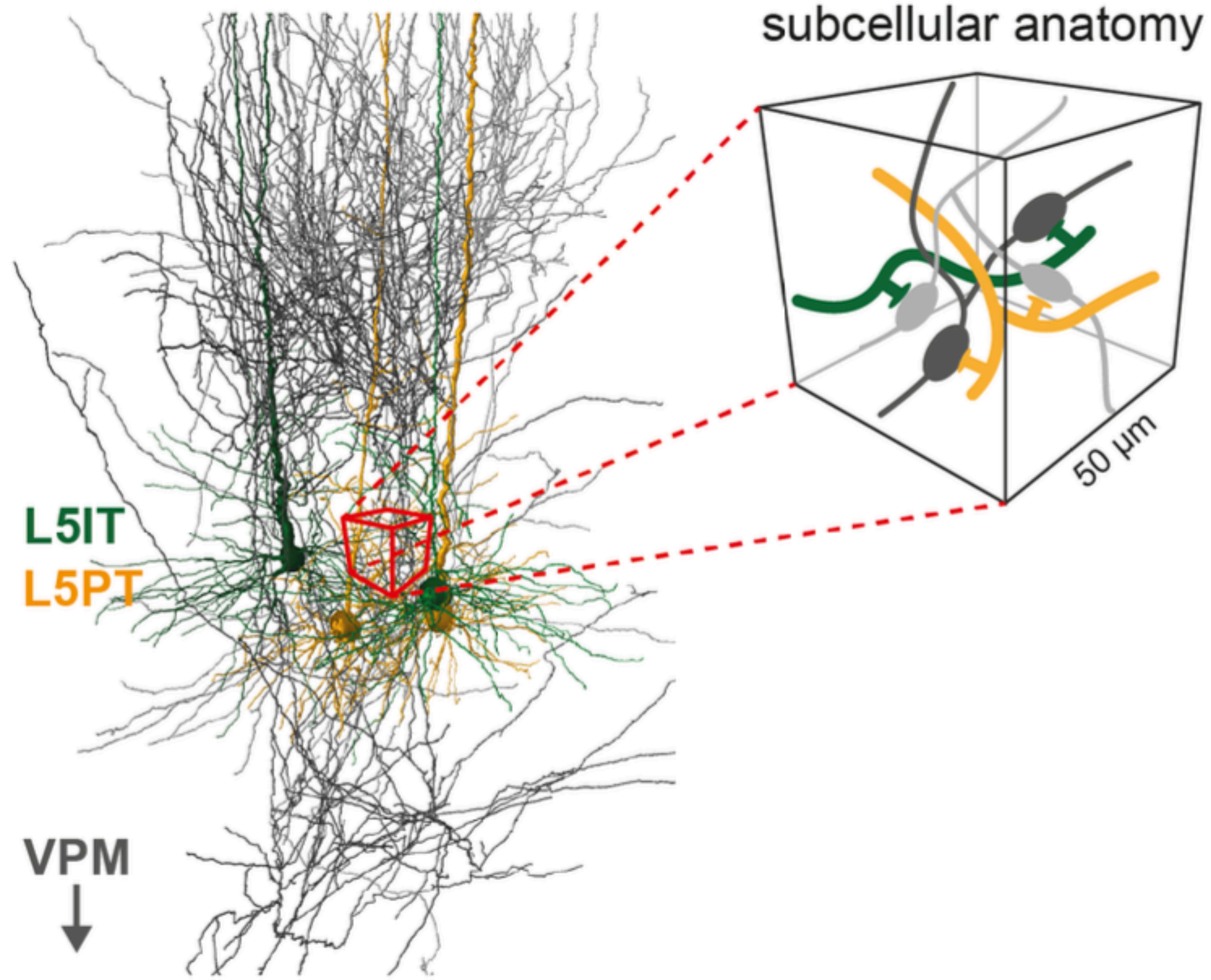


Dense Structural Overlap (DSO)

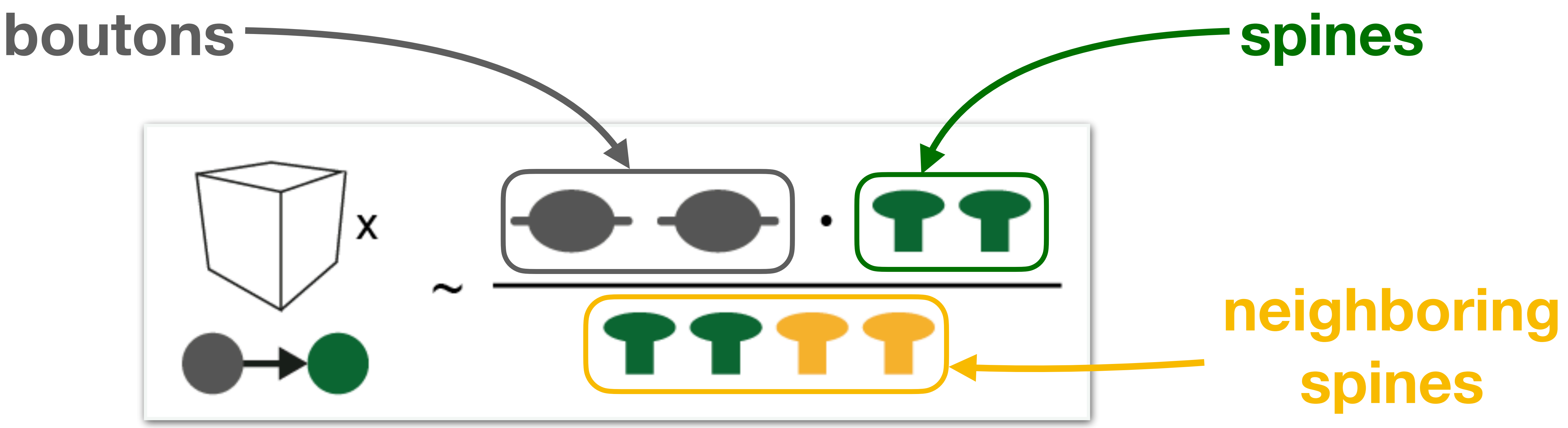
$$\mathrm{DSO}_{i,j,k}(\theta) = \frac{pre_i^{\theta_{pre}} \cdot post_j^{\theta_{post}}}{postAll_k^{\theta_{postAll}}}$$

Boelts et al. 2023; Udvary et al. 2022

A structural wiring rule for the barrel cortex



Thalamus



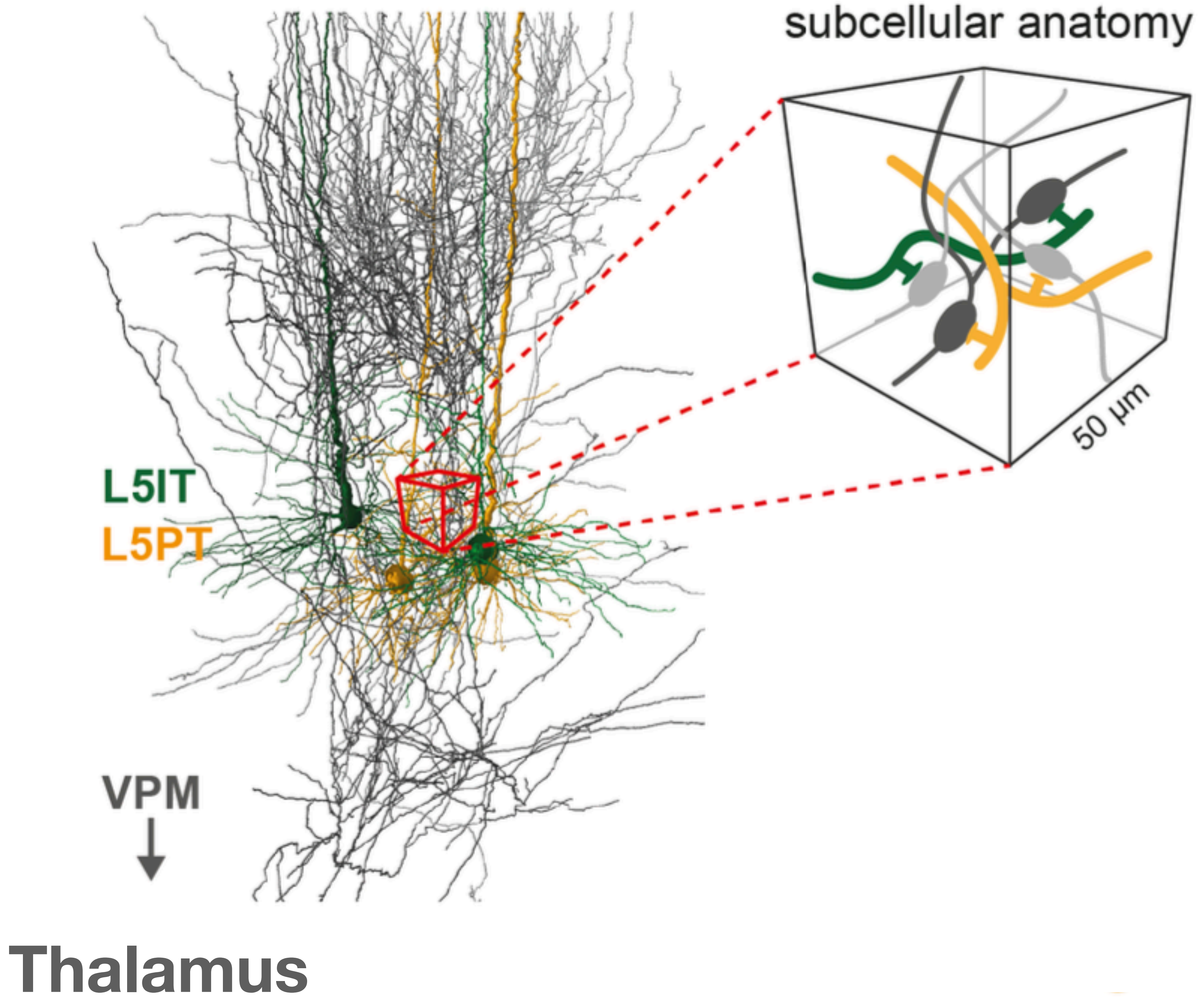
Dense Structural Overlap (DSO)

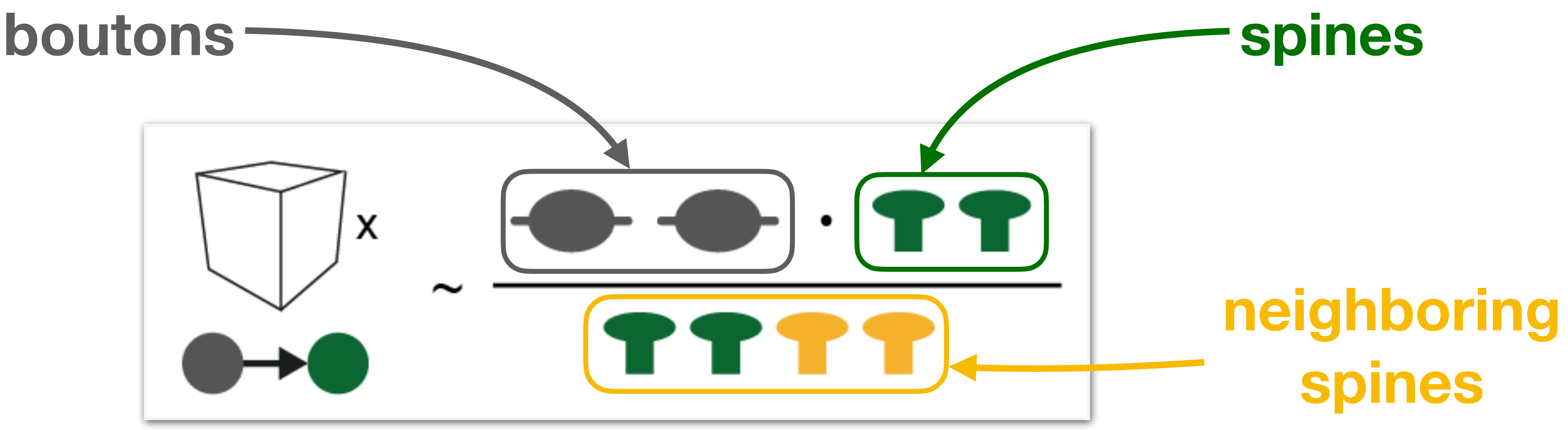
$$\mathrm{DSO}_{i,j,k}(\theta) = \frac{pre_i^{\theta_{pre}} \cdot post_j^{\theta_{post}}}{postAll_k^{\theta_{postAll}}}$$

- Calculate DSO for every neuron pair in the model

Boelts et al. 2023; Udvary et al. 2022

A structural wiring rule for the barrel cortex





Dense Structural Overlap (DSO)

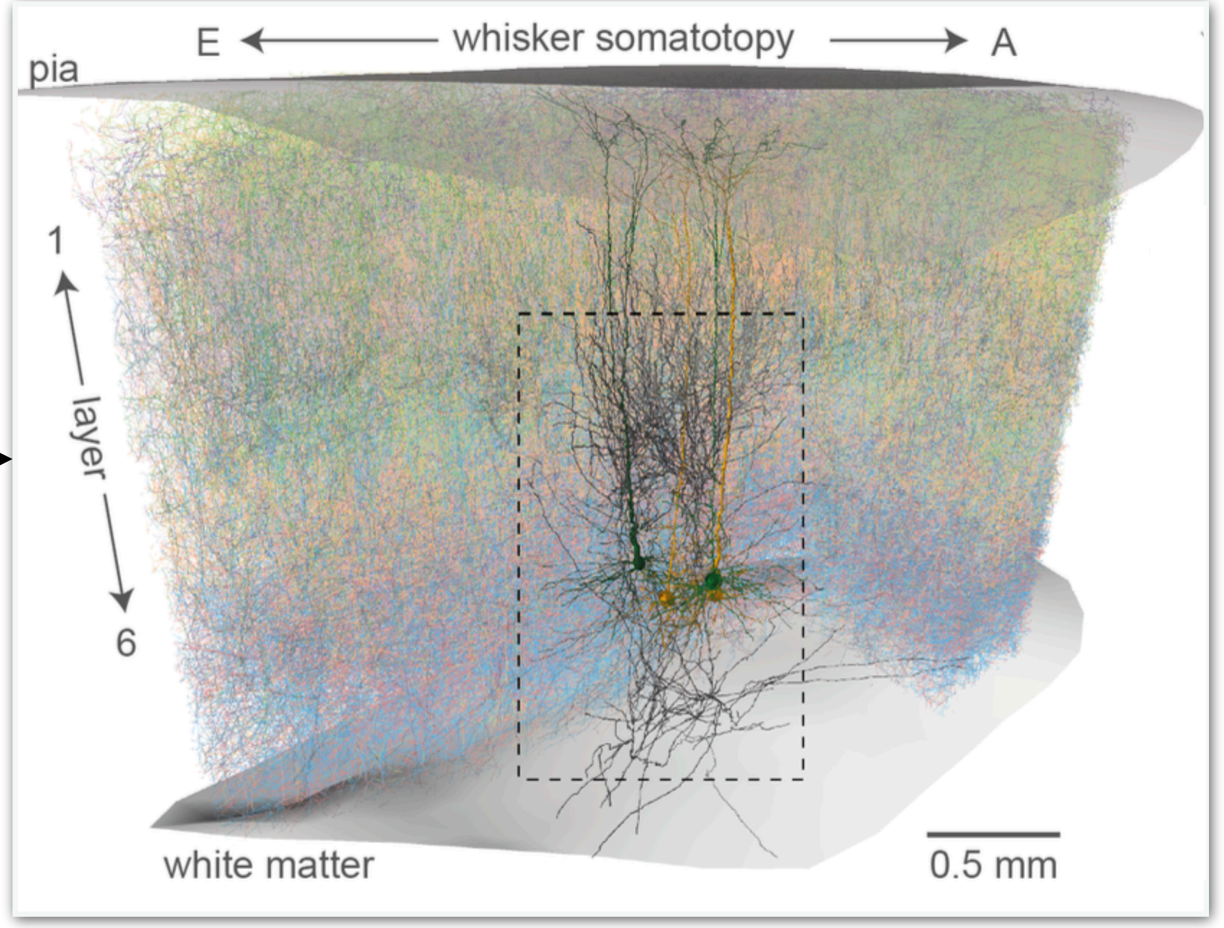
$$\mathrm{DSO}_{i,j,k}(\theta) = \frac{pre_i^{\theta_{pre}} \cdot post_j^{\theta_{post}}}{postAll_k^{\theta_{postAll}}}$$

- Calculate DSO for every neuron pair in the model
- Draw connections from DSO probabilities: $c \sim$ Poisson(DSO(θ))

Boelts et al. 2023; Udvary et al. 2022

Testing the DSO rule with empirical data

$$\text{DSO}_{i,j,k}(\theta) = \frac{pre_i^{\theta_{pre}} \cdot post_j^{\theta_{post}}}{postAll_k^{\theta_{postAll}}}$$



Boelts et al. 2023; Bruno & Sakmann, 2006; Constantinopel & Bruno, 2013

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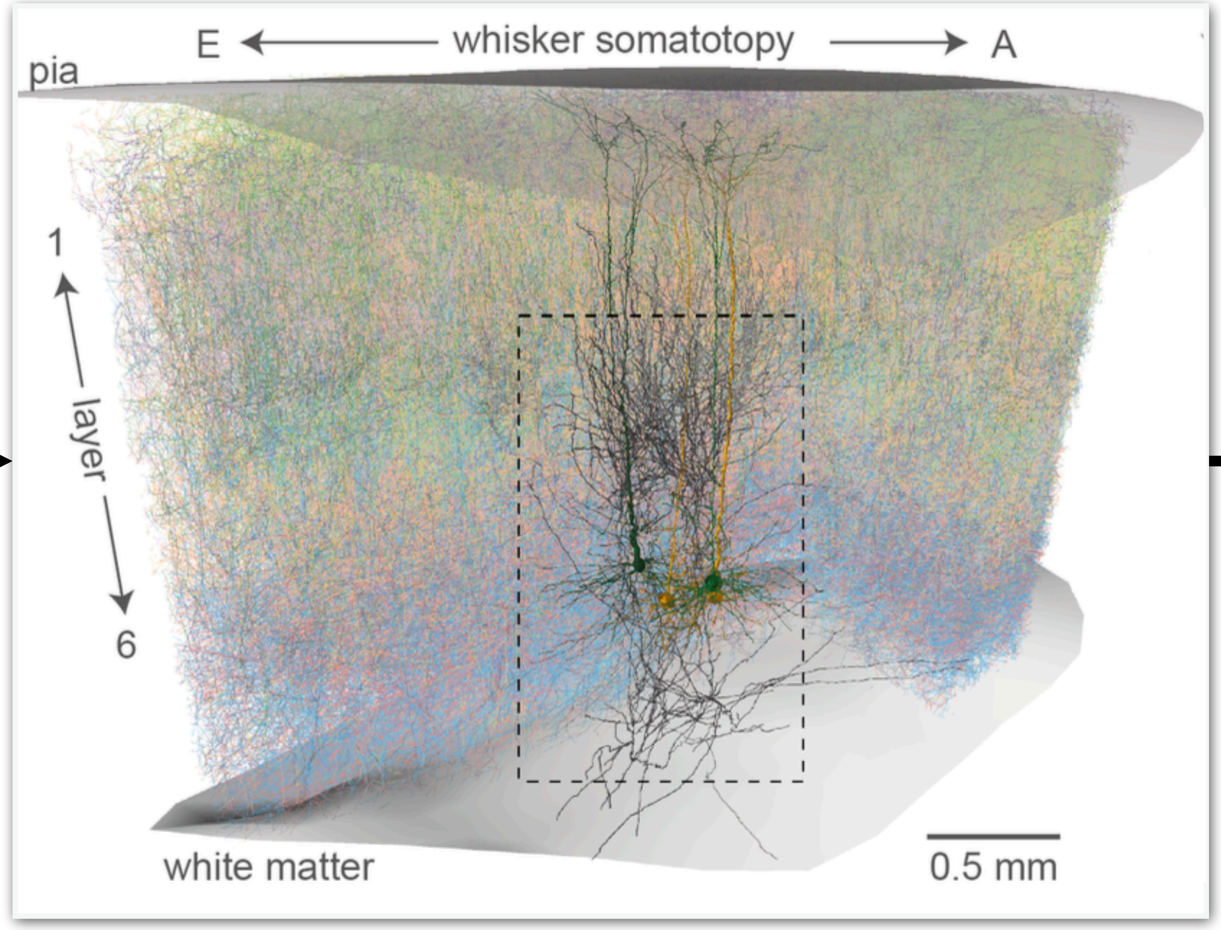

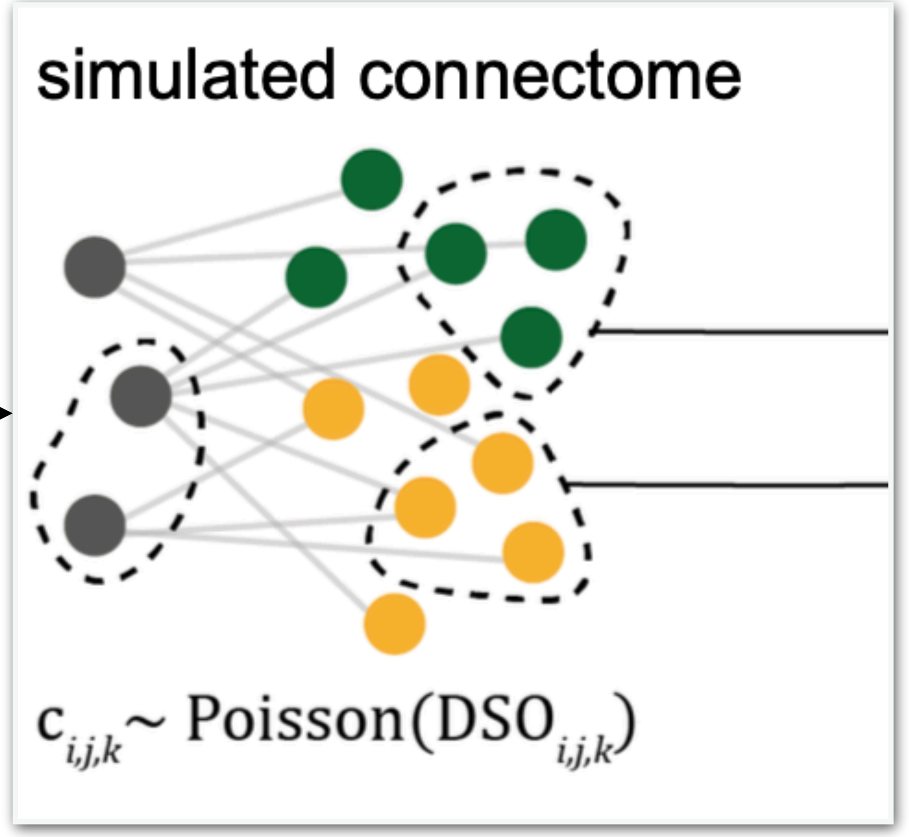

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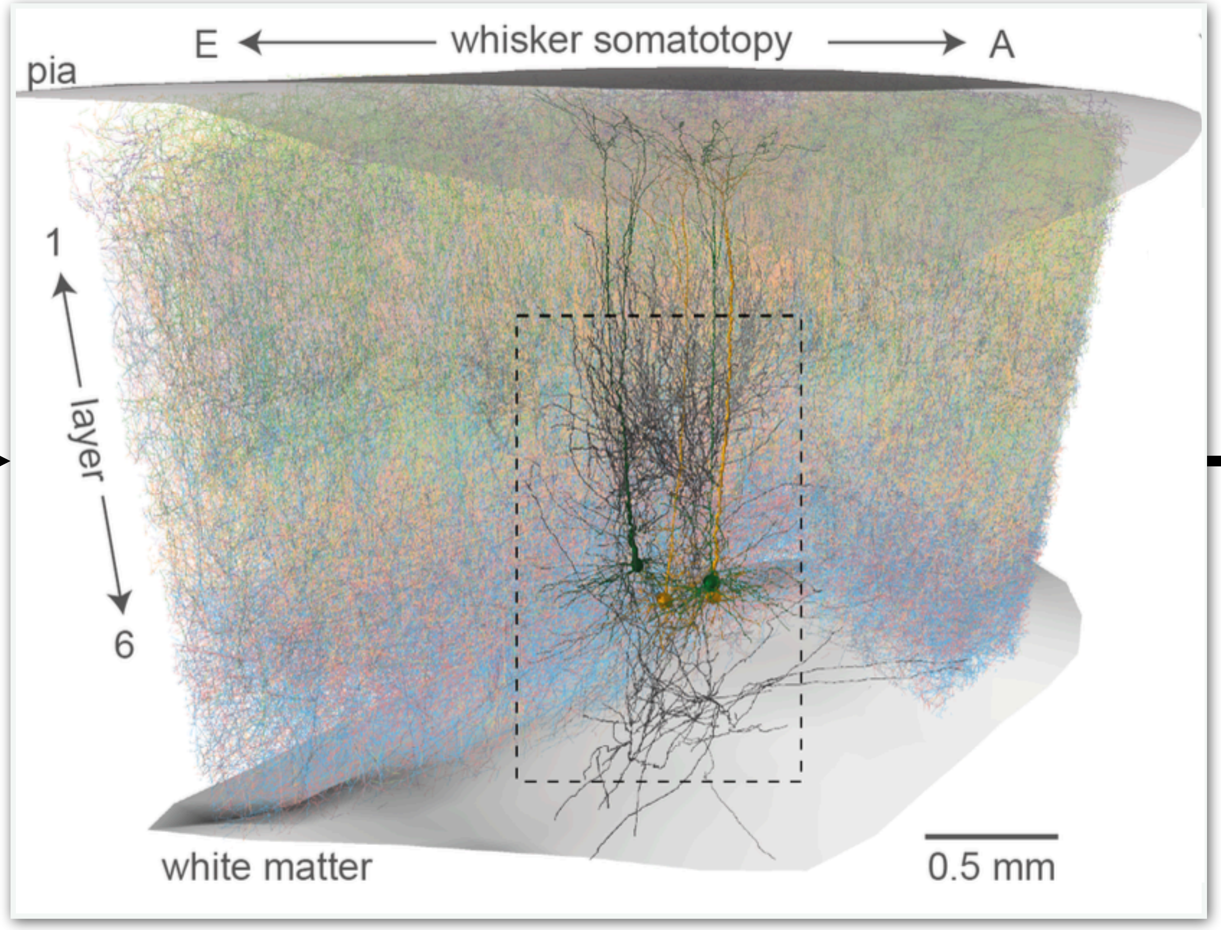
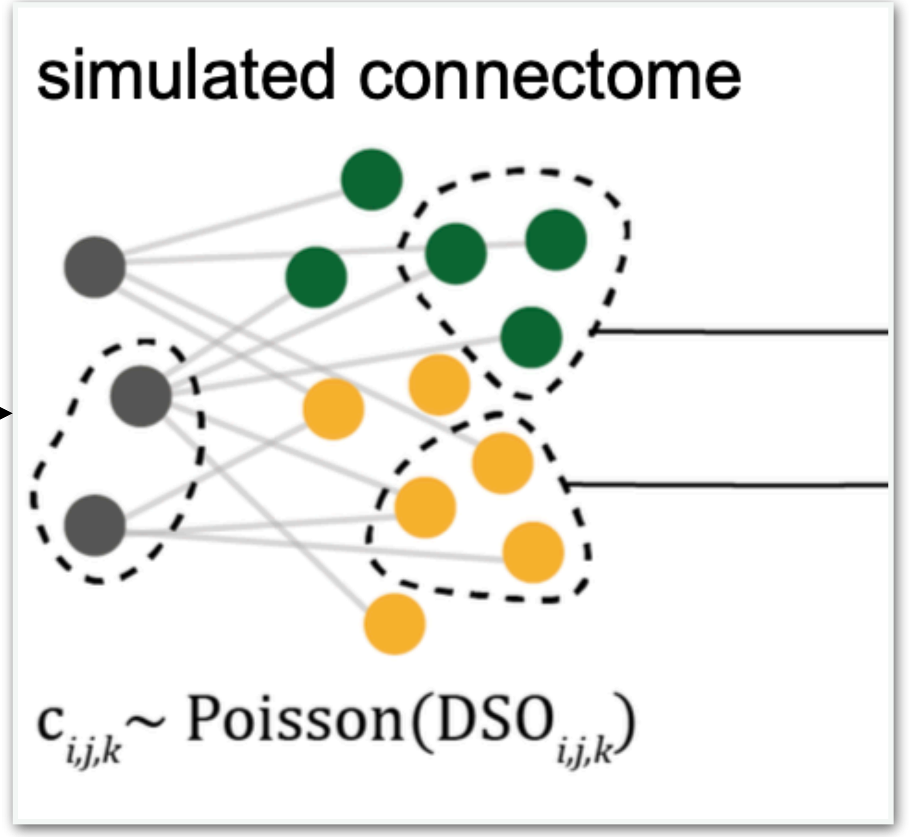




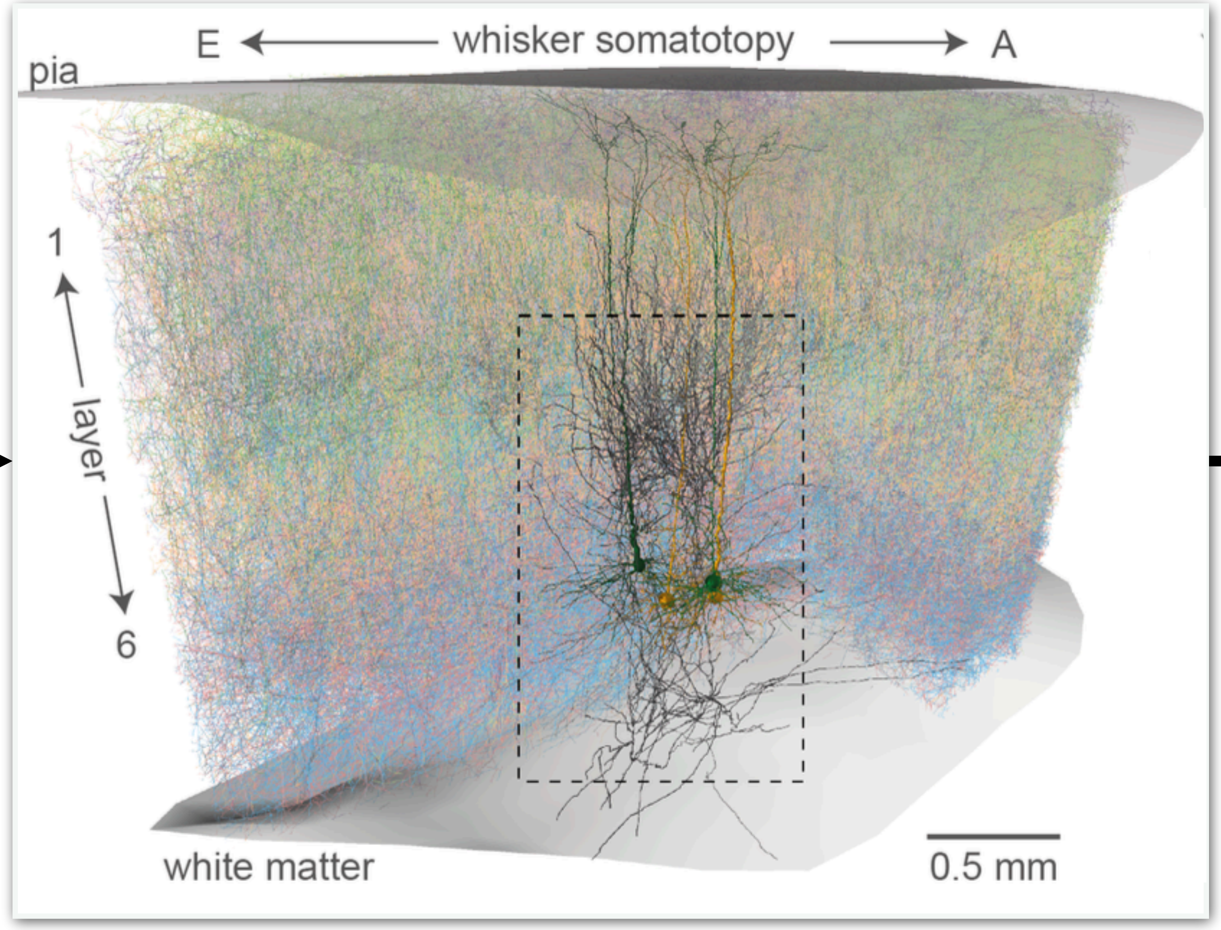
Which empirical data do we have for the barrel cortex?

Boelts et al. 2023; Bruno & Sakmann, 2006; Constantinopel & Bruno, 2013

Testing the DSO rule with empirical data

$$\mathrm{DSO}_{i,j,k}(\theta) = \frac{pre_i^{\theta_{pre}} \cdot post_j^{\theta_{post}}}{postAll_k^{\theta_{postAll}}}$$

→



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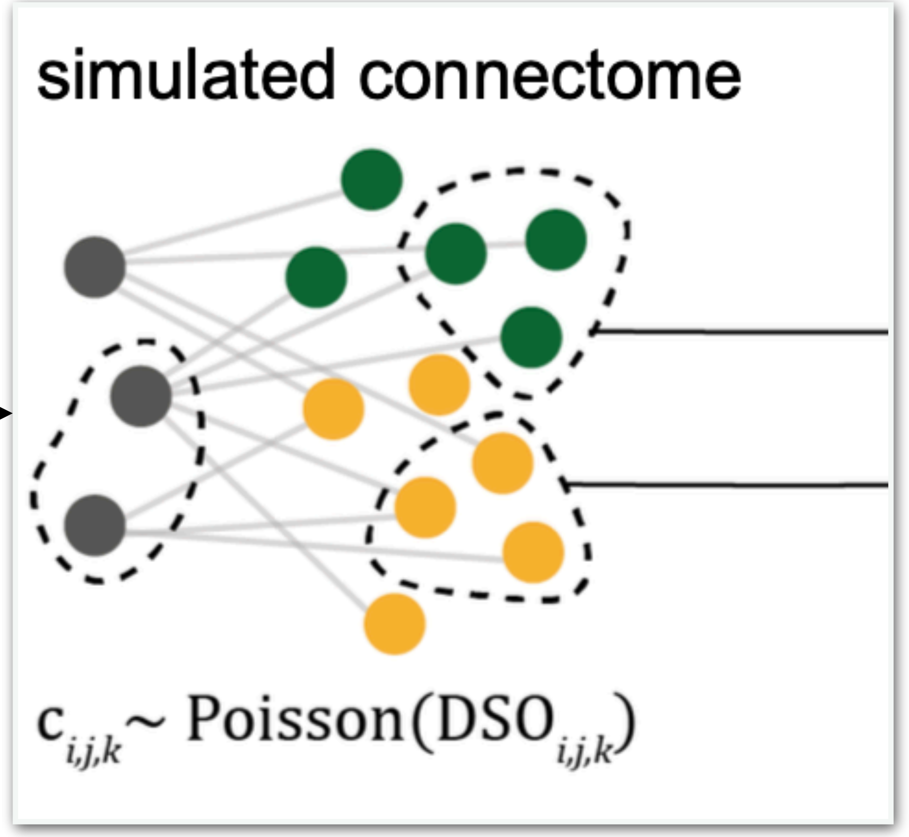

Which empirical data do we have for the barrel cortex?

Connection counts from paired recordings

Boelts et al. 2023; Bruno & Sakmann, 2006; Constantinopel & Bruno, 2013

Testing the DSO rule with empirical data

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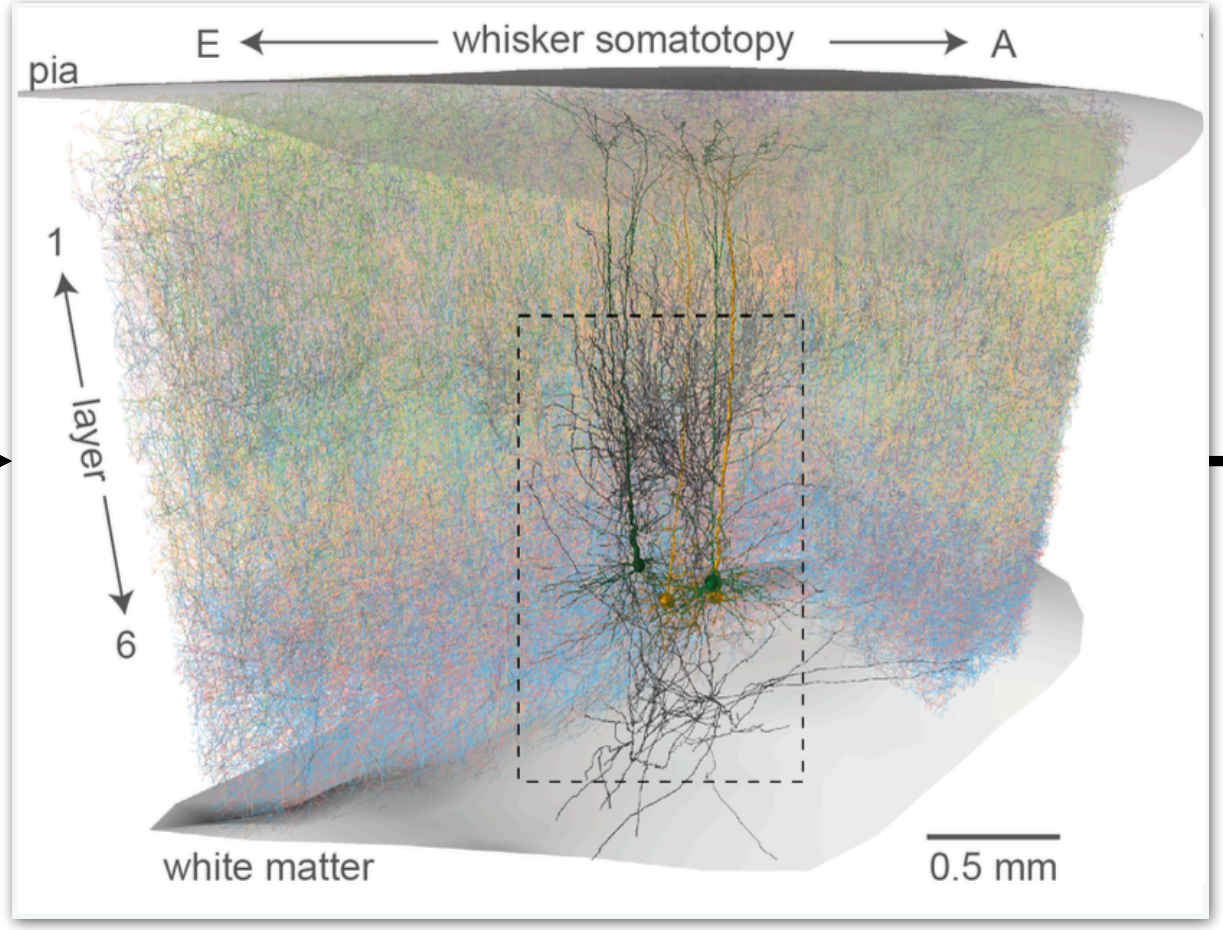

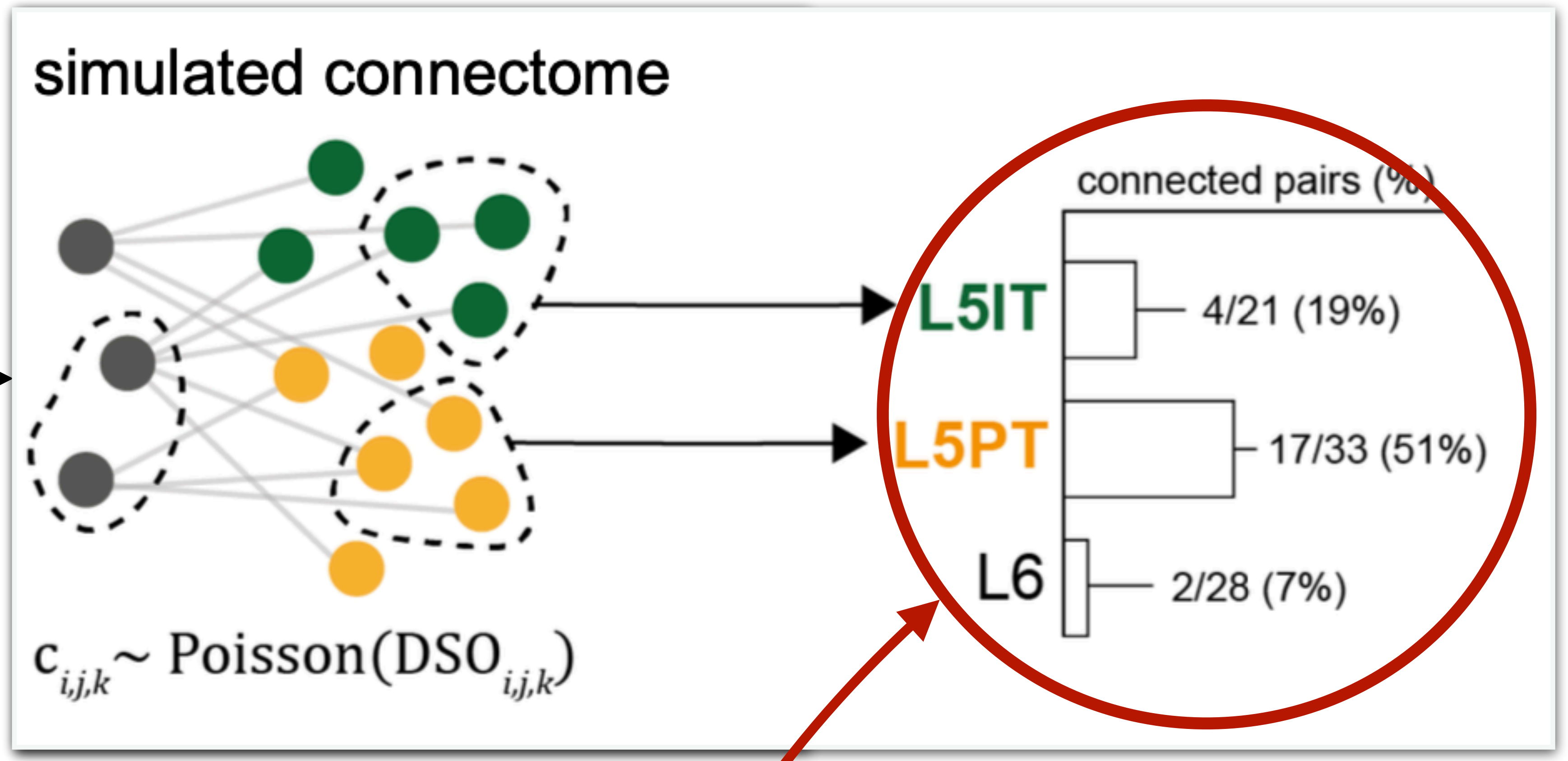

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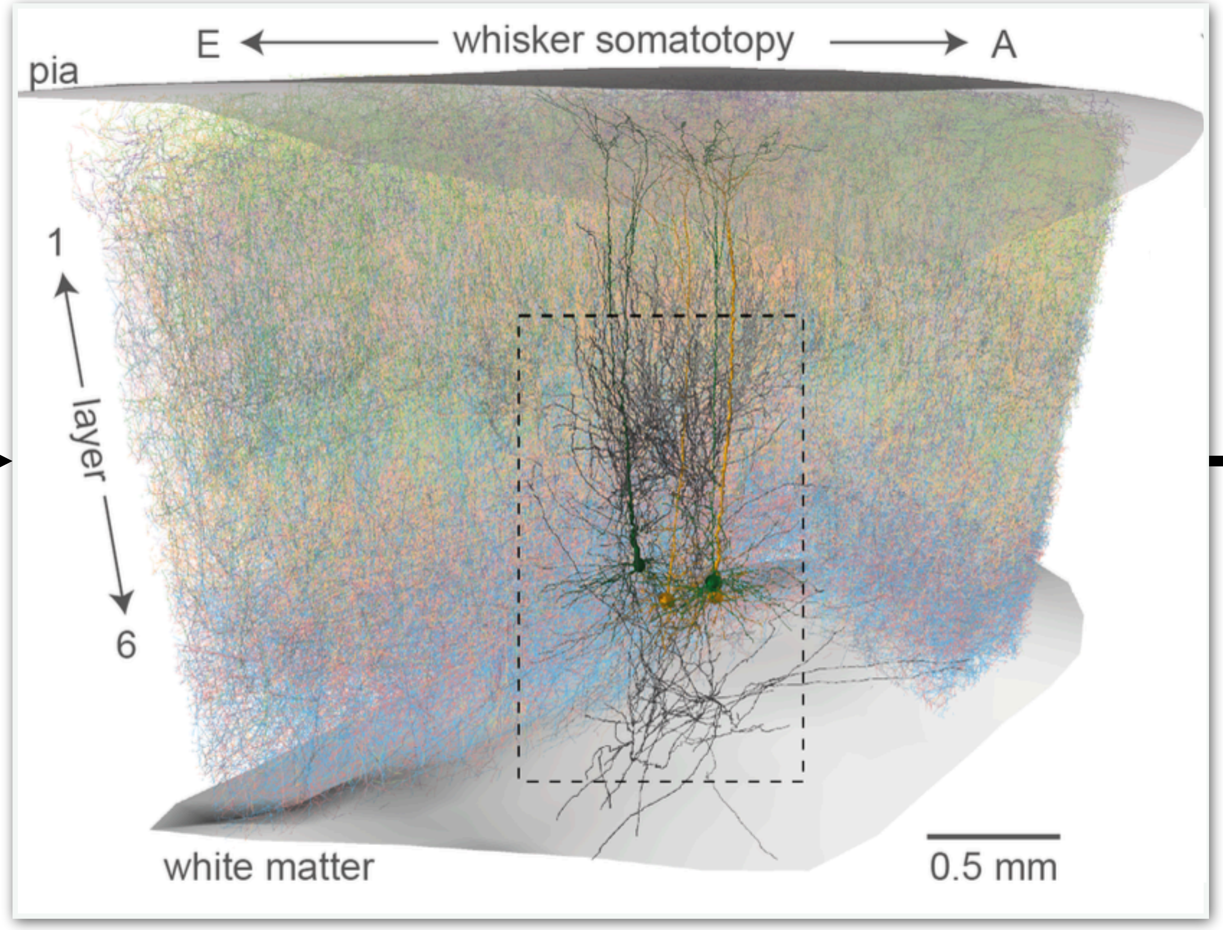
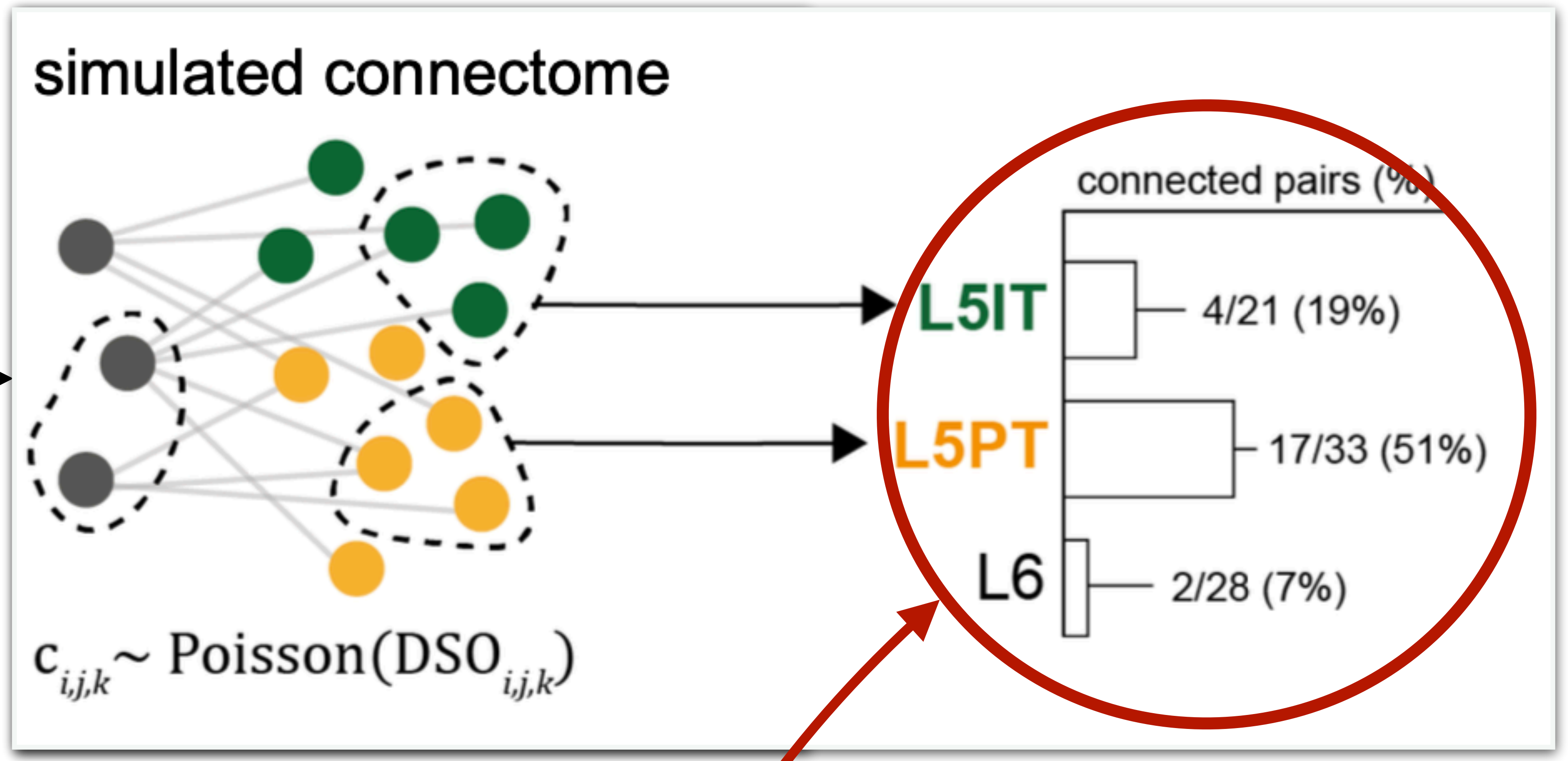
$$\mathrm{DSO}_{i,j,k}(\theta) = \frac{pre_i^{\theta_{pre}} \cdot post_j^{\theta_{post}}}{postAll_k^{\theta_{postAll}}}$$



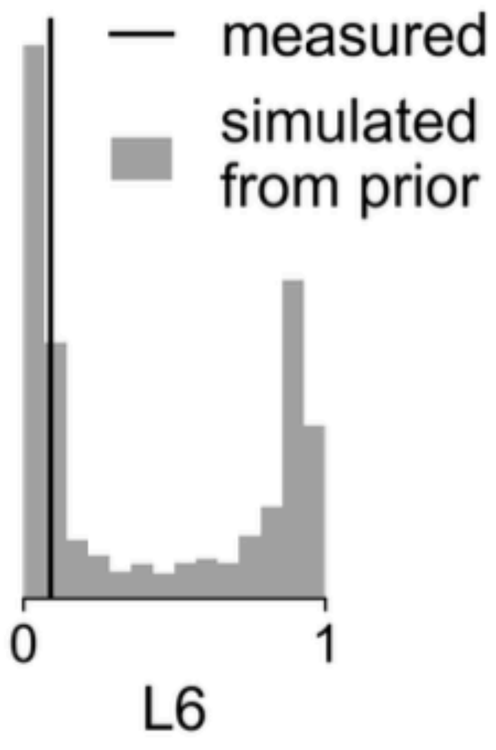


Which empirical data do we have for the barrel cortex?

Connection counts from paired recordings

$\theta_i \sim p(\theta)$

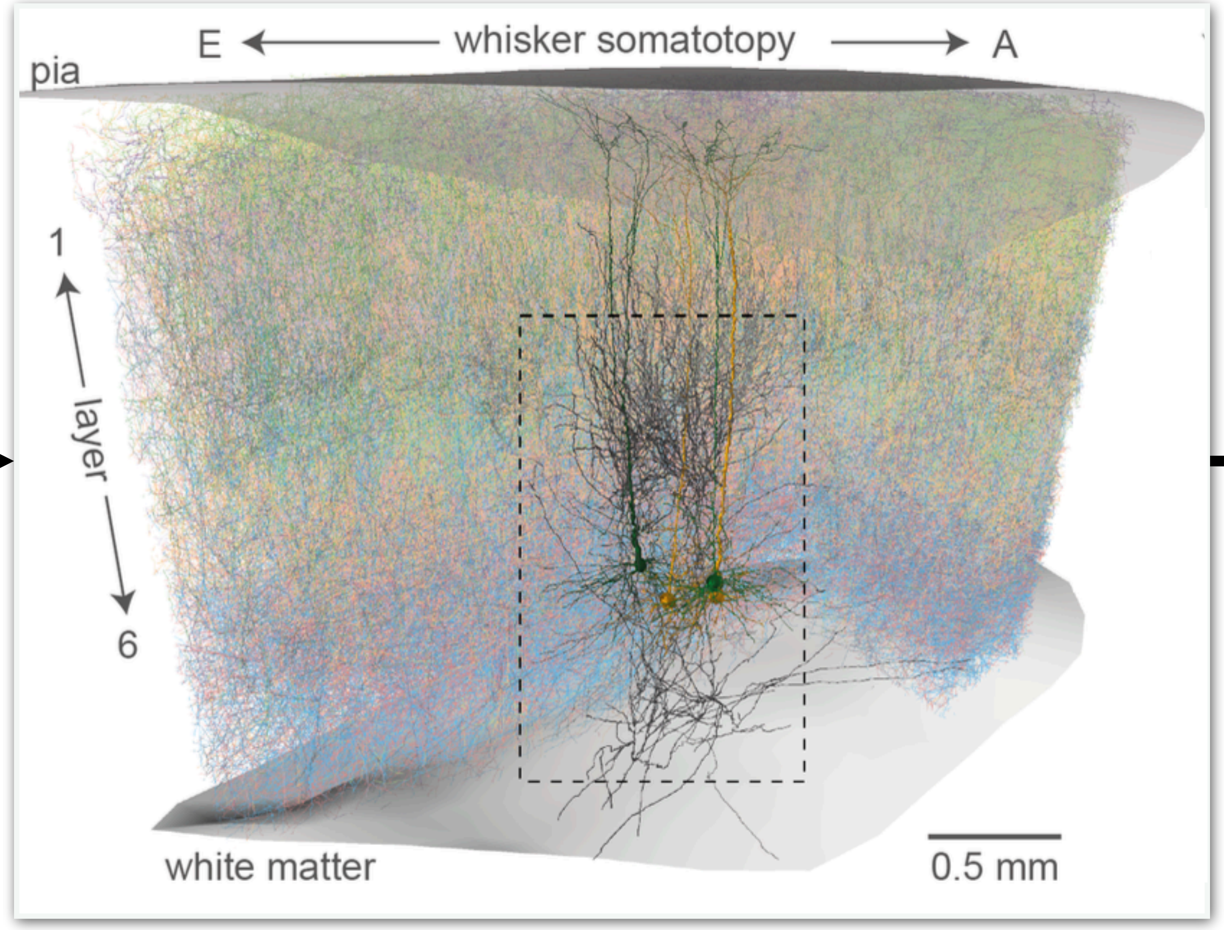
$c(\theta_i) \sim \mathrm{Poisson}(\mathrm{DSO}(\theta_i))$

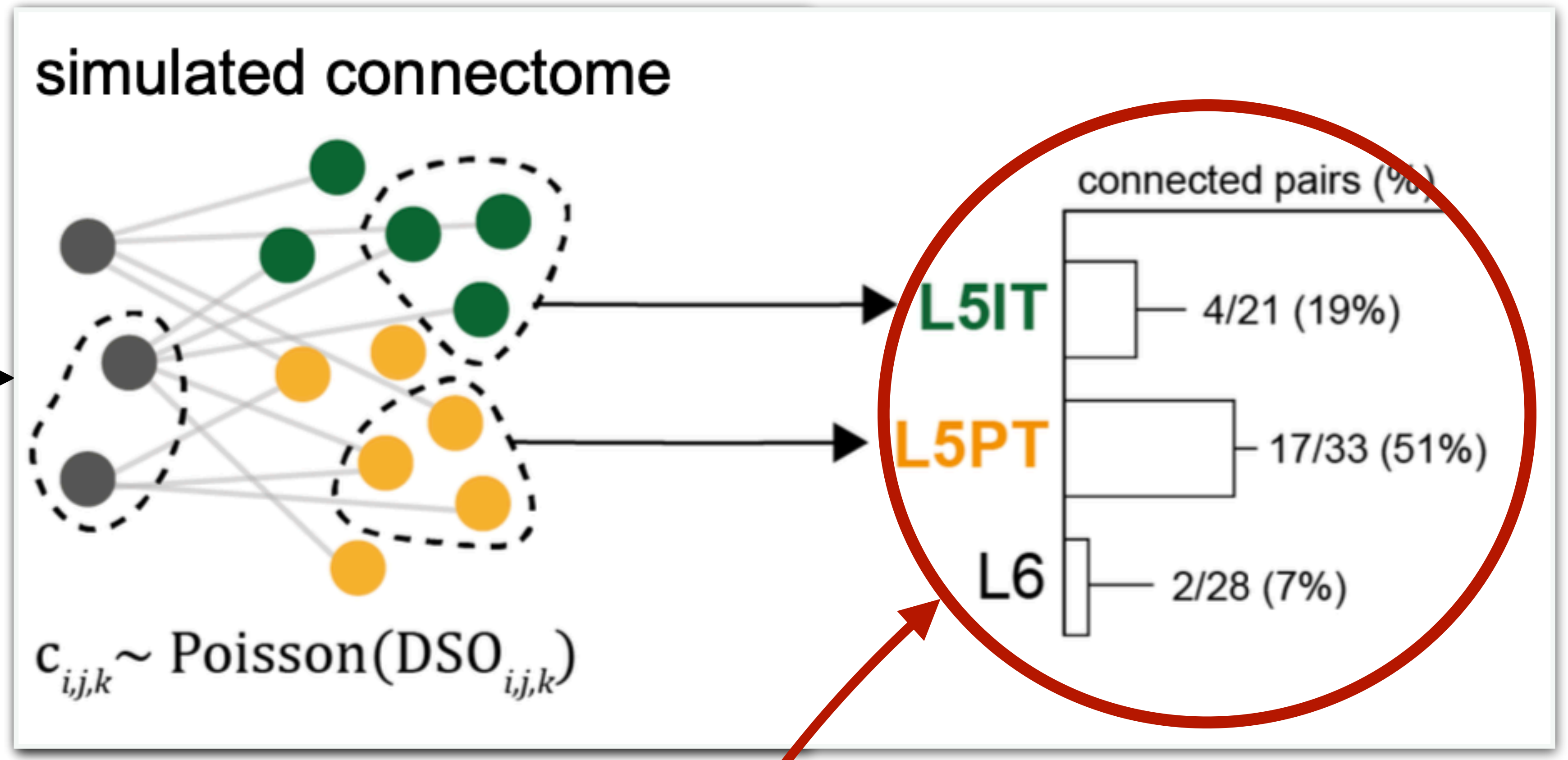


Boelts et al. 2023; Bruno & Sakmann, 2006; Constantinopel & Bruno, 2013

Testing the DSO rule with empirical data

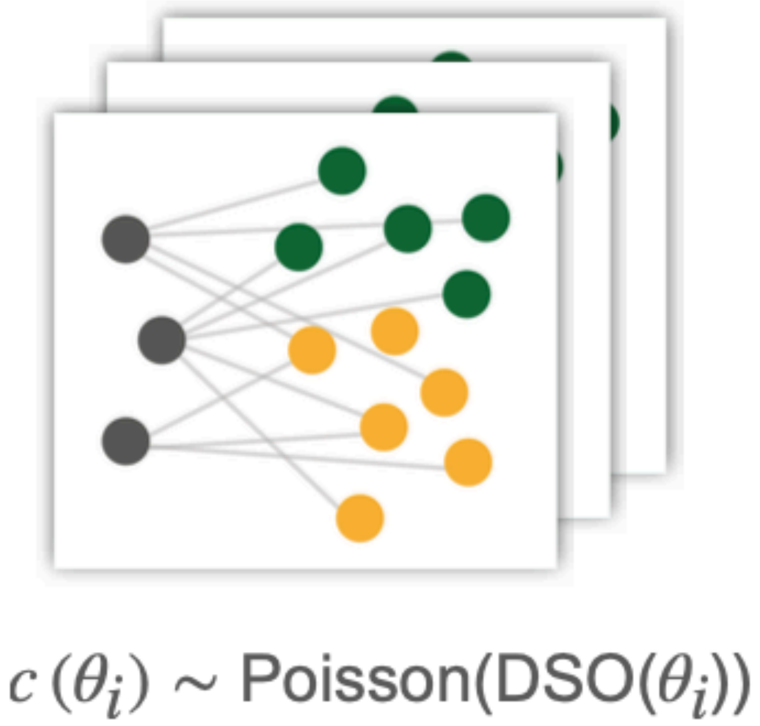
$$\mathrm{DSO}_{i,j,k}(\theta) = \frac{pre_i^{\theta_{pre}} \cdot post_j^{\theta_{post}}}{postAll_k^{\theta_{postAll}}}$$

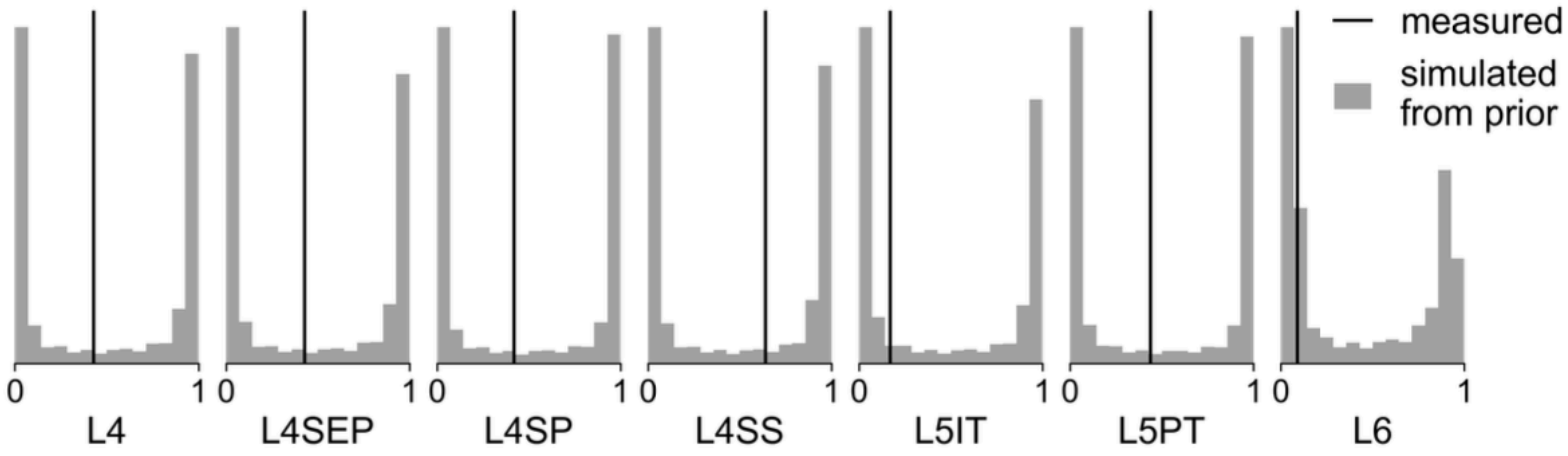




Which empirical data do we have for the barrel cortex?

Connection counts from paired recordings



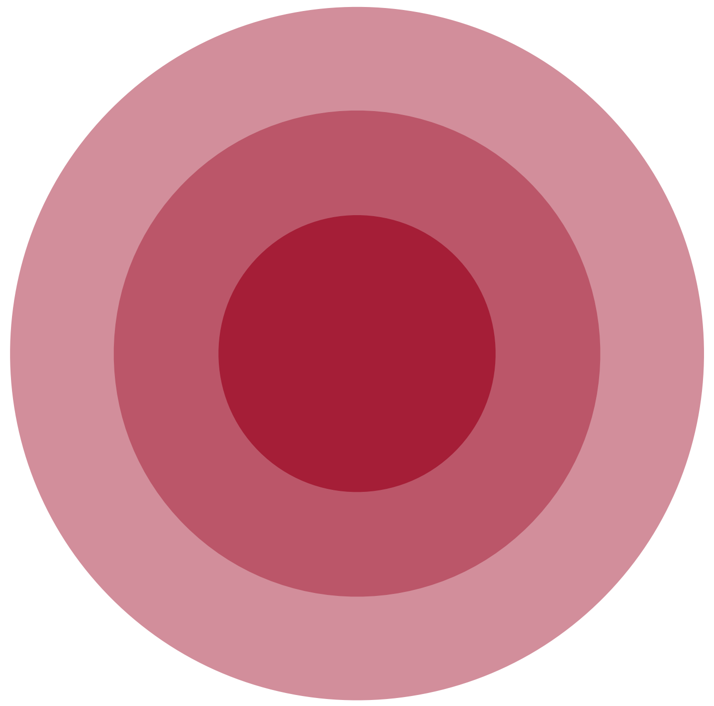


Boelts et al. 2023; Bruno & Sakmann, 2006; Constantinopel & Bruno, 2013

Bayesian inference for wiring rules

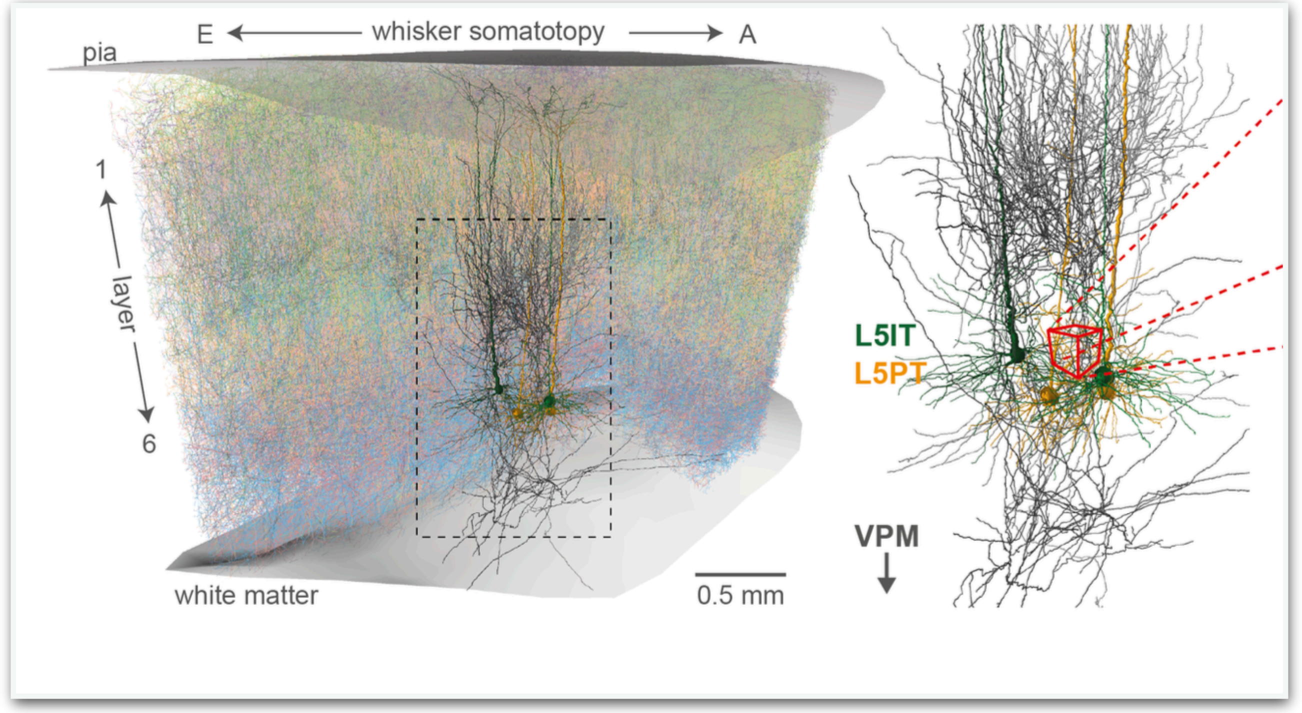
forward model

parameters θ



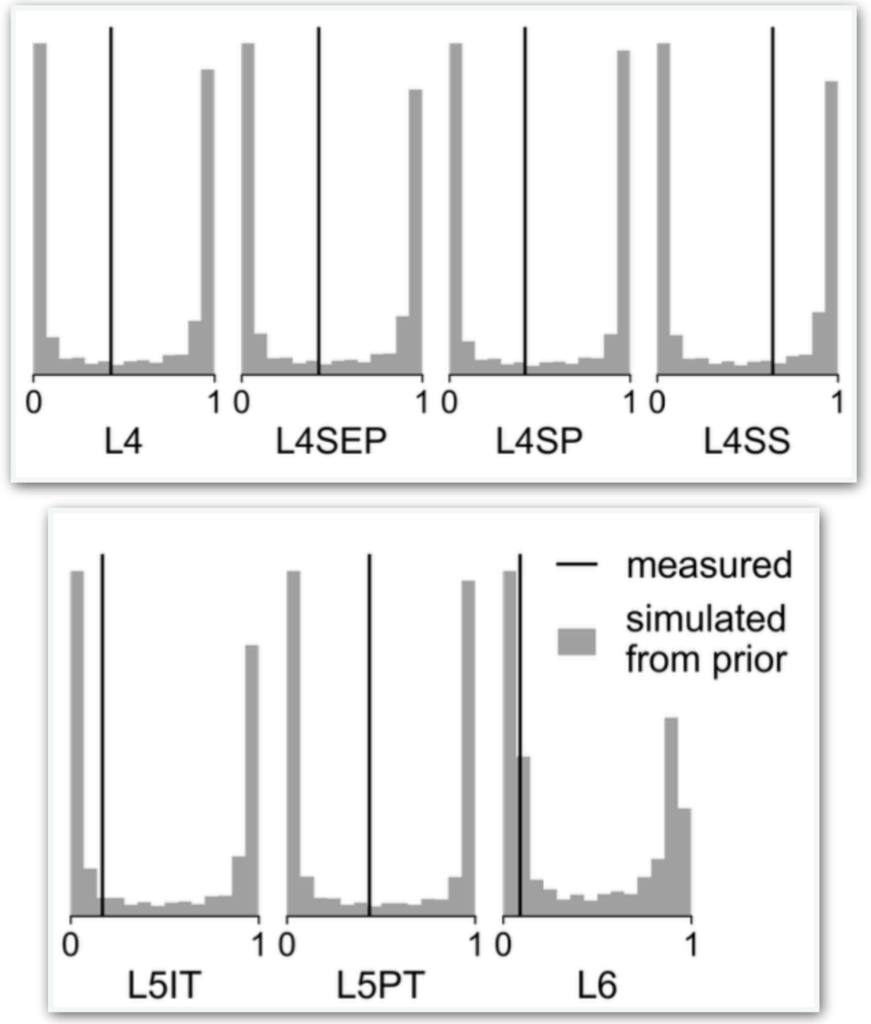
$\theta \sim p(\theta)$

$$\mathrm{DSO}_{i,j,k}(\boldsymbol{\theta}) = \frac{pre_i^{\theta_{pre}} \cdot post_j^{\theta_{post}}}{postAll_k^{\theta_{postAll}}}$$



$$p(\theta \mid x) \propto p(x \mid \theta)\, p(\theta)$$

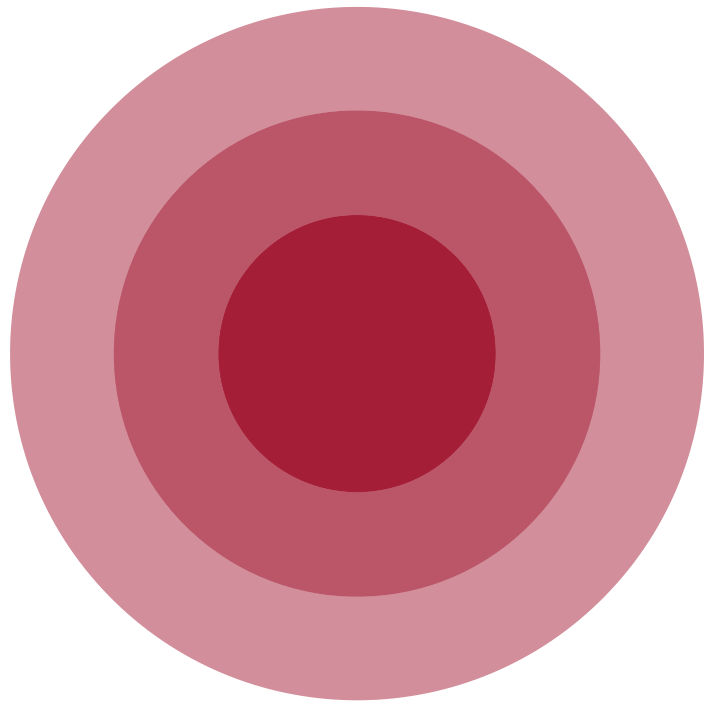
data x



Bayesian inference for wiring rules

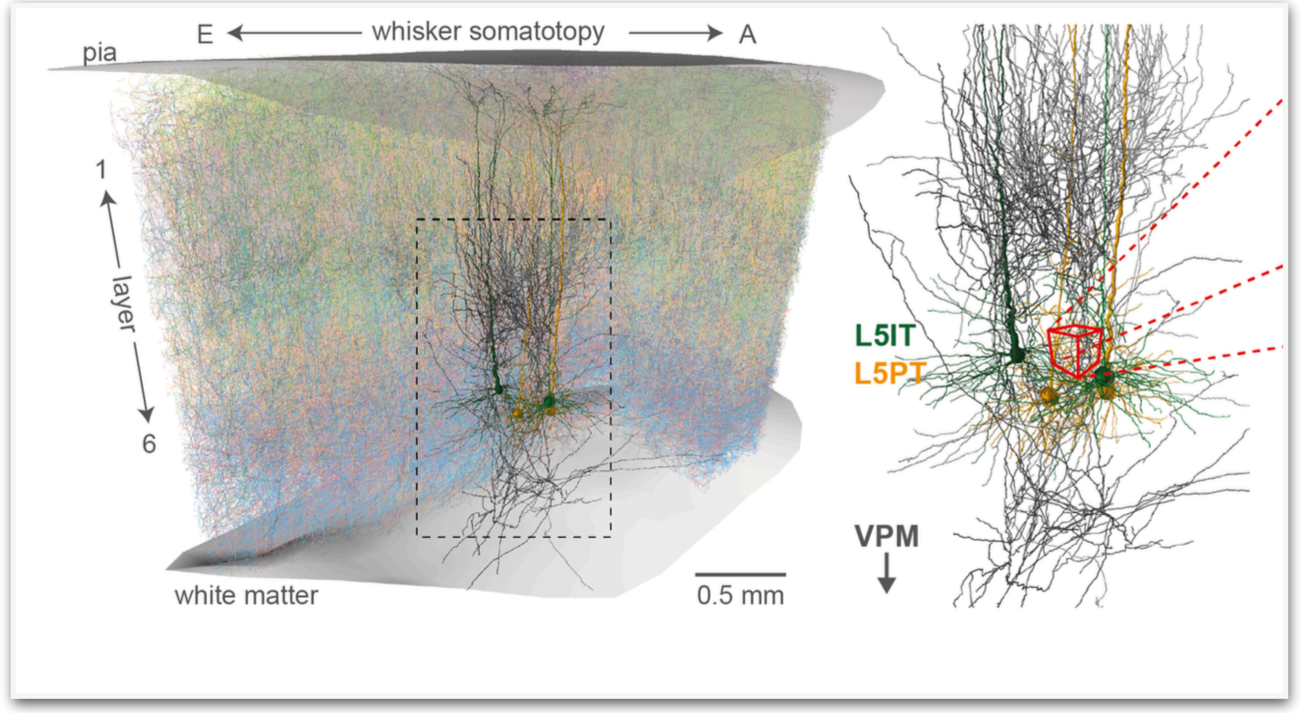
forward model

parameters θ



$\theta \sim p(\theta)$

$$\mathrm{DSO}_{i,j,k}(\boldsymbol{\theta}) = \frac{pre_i^{\theta_{pre}} \cdot post_j^{\theta_{post}}}{postAll_k^{\theta_{postAll}}}$$



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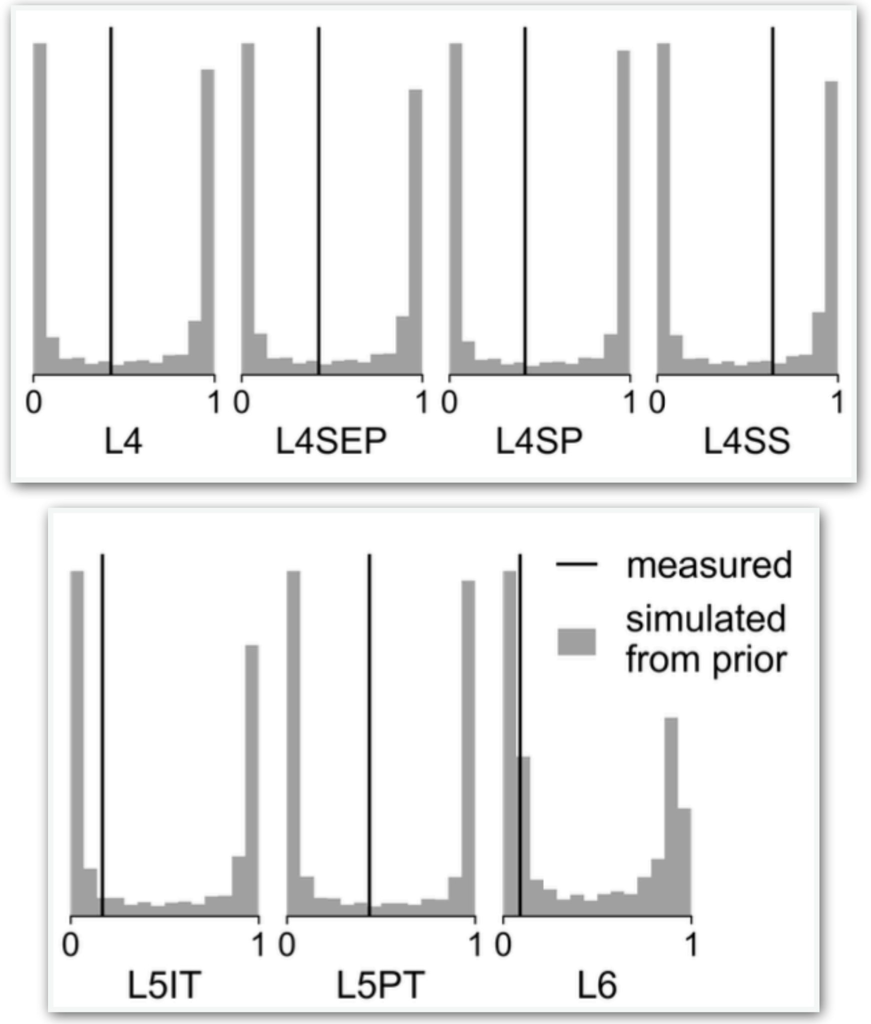
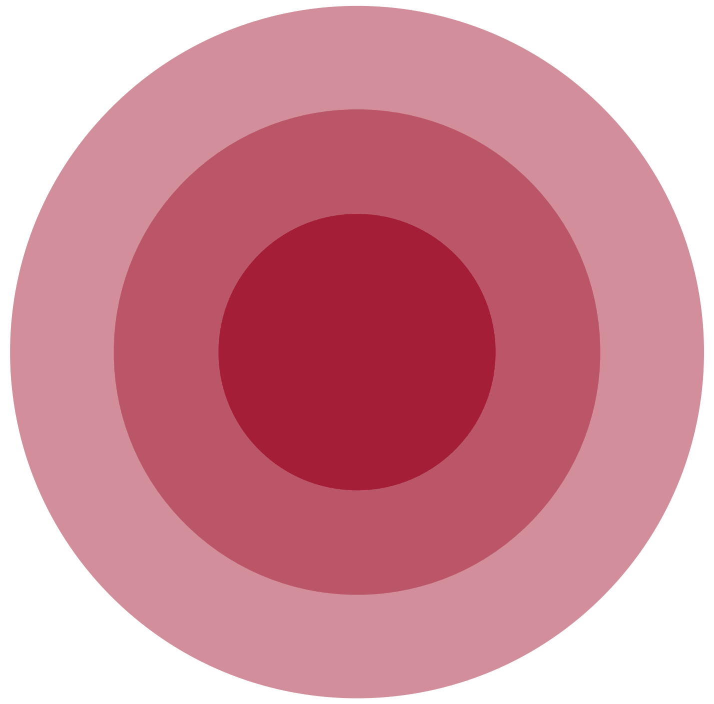
data x



Bayesian inference for wiring rules

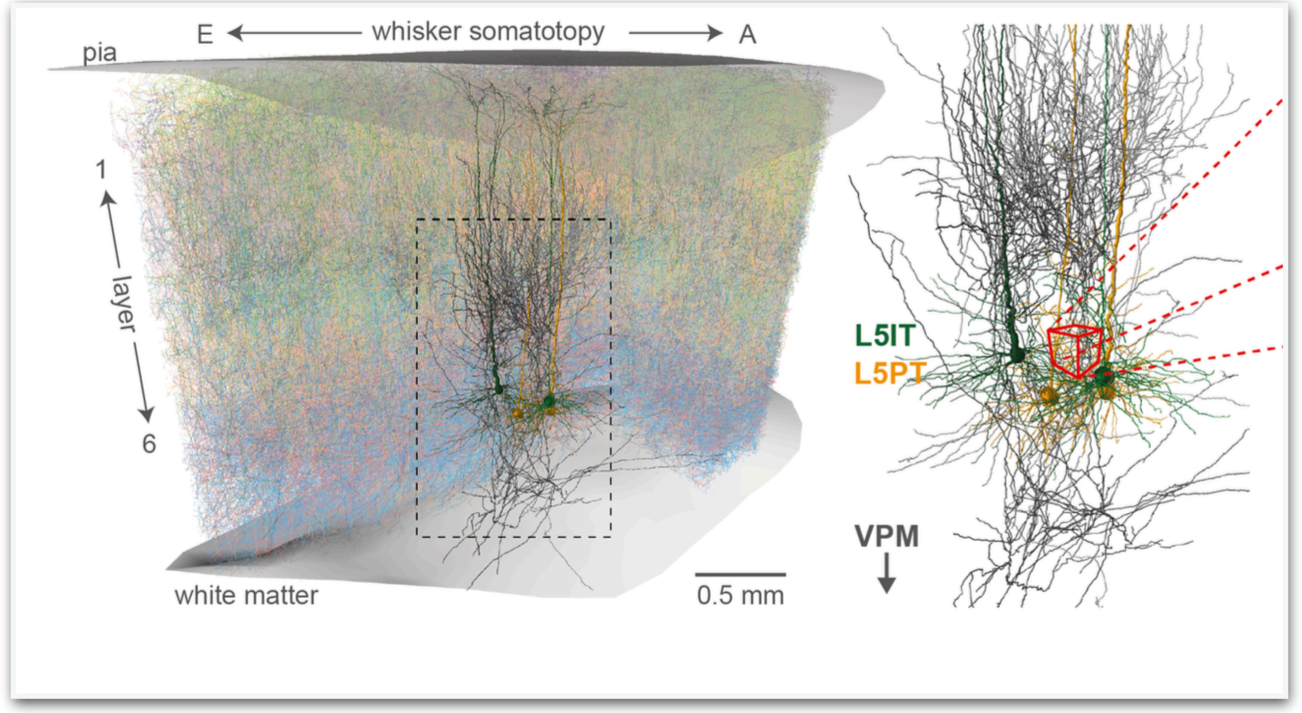
forward model

parameters θ

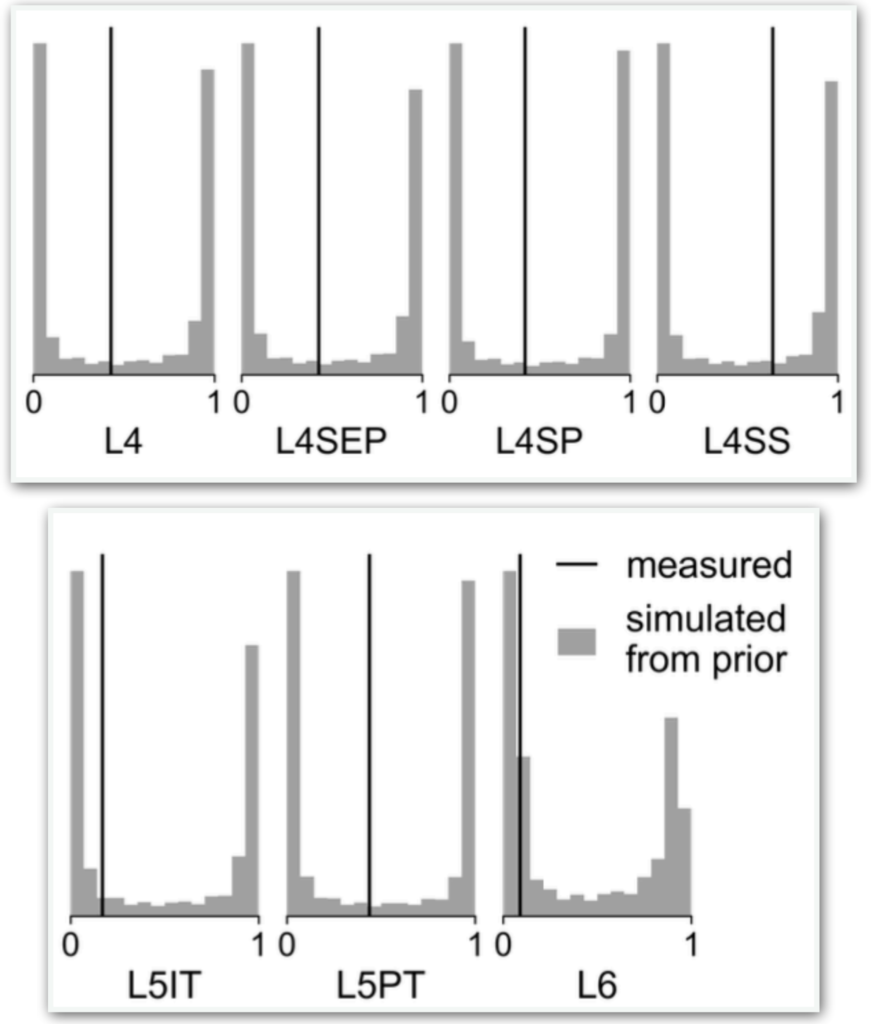


$\theta \sim p(\theta)$

$$\mathrm{DSO}_{i,j,k}(\boldsymbol{\theta}) = \frac{pre_i^{\theta_{pre}} \cdot post_j^{\theta_{post}}}{postAll_k^{\theta_{postAll}}}$$

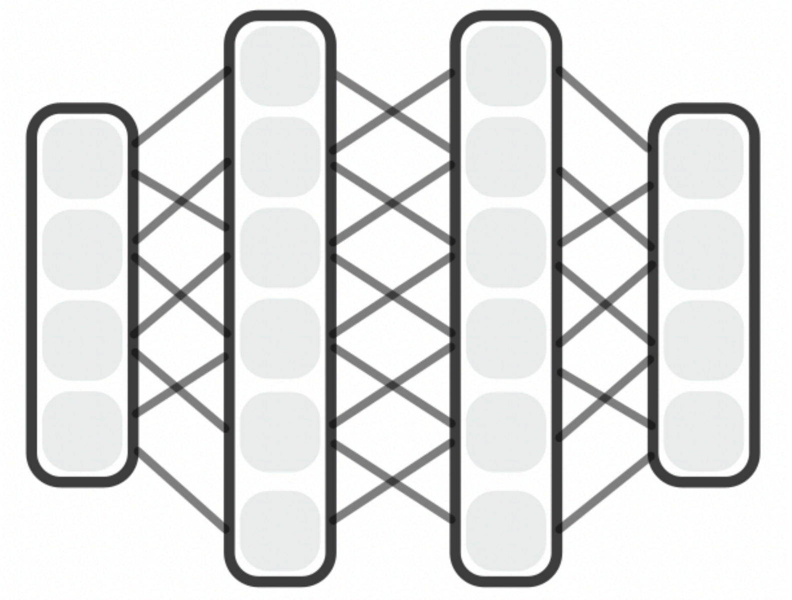


data x



$$p(\theta \mid x) \propto p(x \mid \theta)\, p(\theta)$$

simulation-based inference



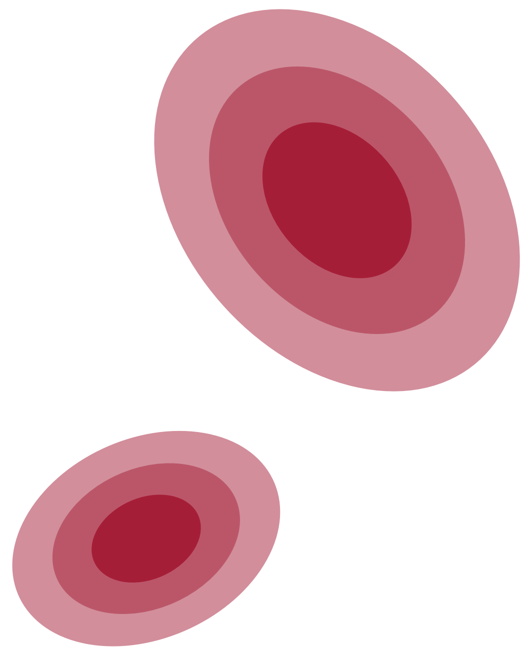
training data

$\{(\theta_1, x_1), (\theta_2, x_2), \ldots\}$

Bayesian inference for wiring rules

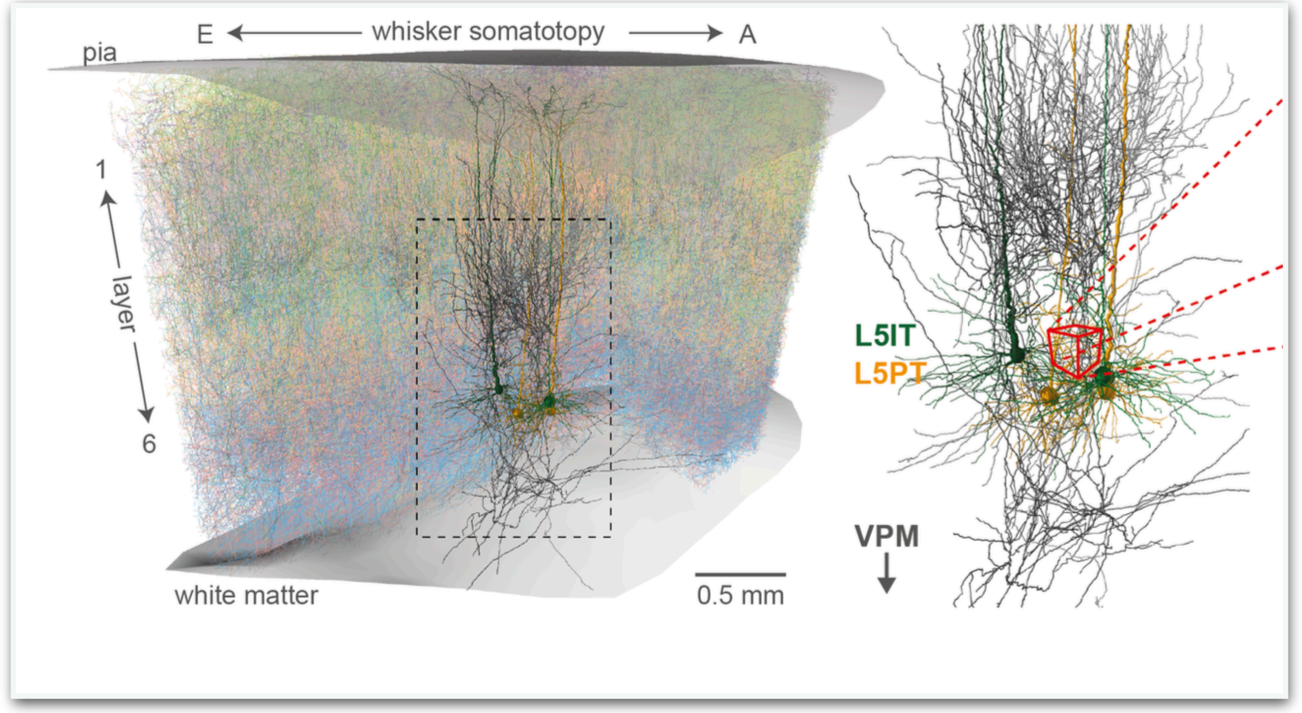
forward model

parameters θ

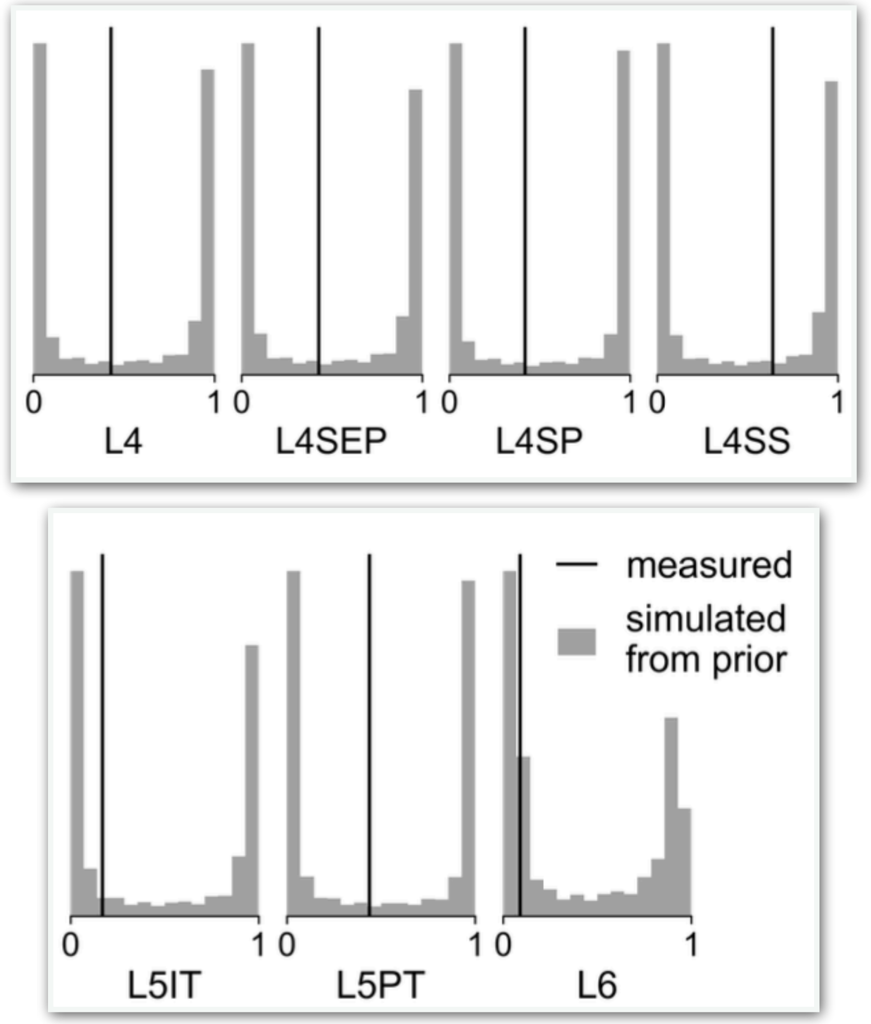


$p(\theta | x)$

$$\mathrm{DSO}_{i,j,k}(\boldsymbol{\theta}) = \frac{pre_i^{\theta_{pre}} \cdot post_j^{\theta_{post}}}{postAll_k^{\theta_{postAll}}}$$

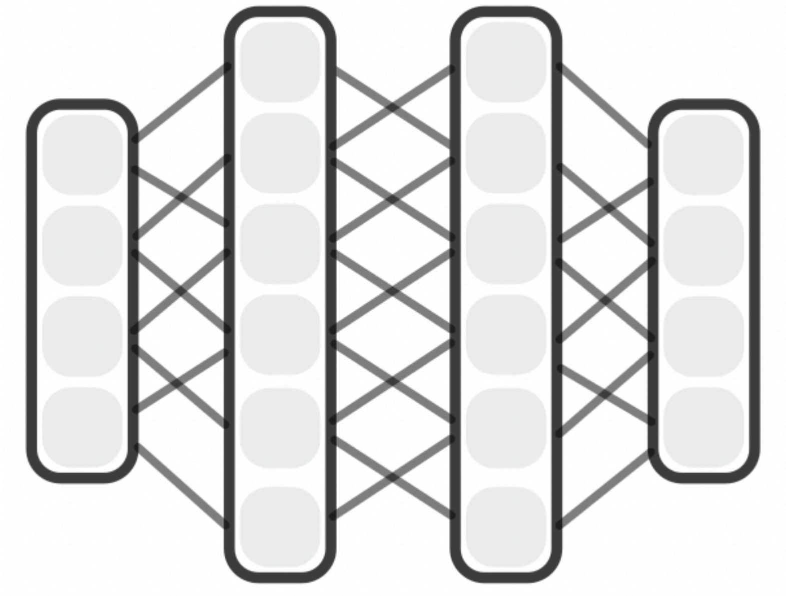


data x



$$p(\theta | x) \propto p(x | \theta) p(\theta)$$

simulation-based inference

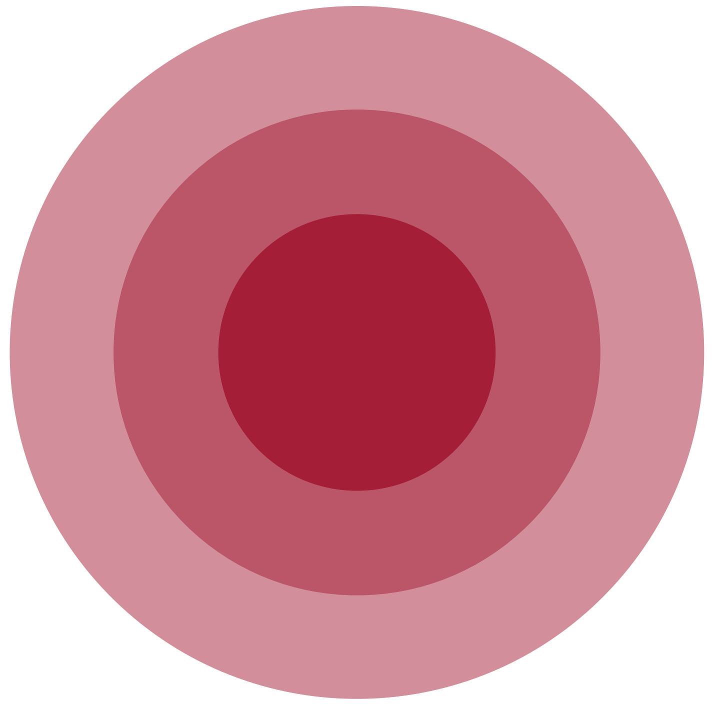


training data

$\{(\theta_1, x_1), (\theta_2, x_2), \ldots\}$

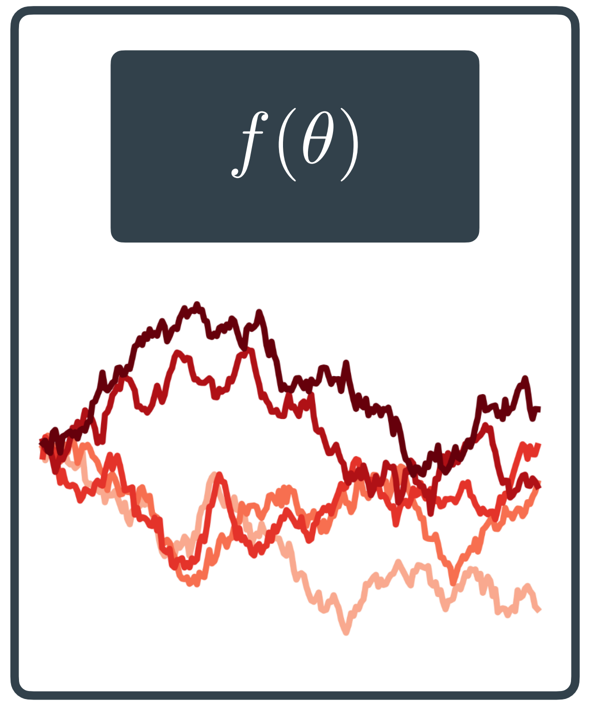
Neural Posterior Estimation (NPE)

prior



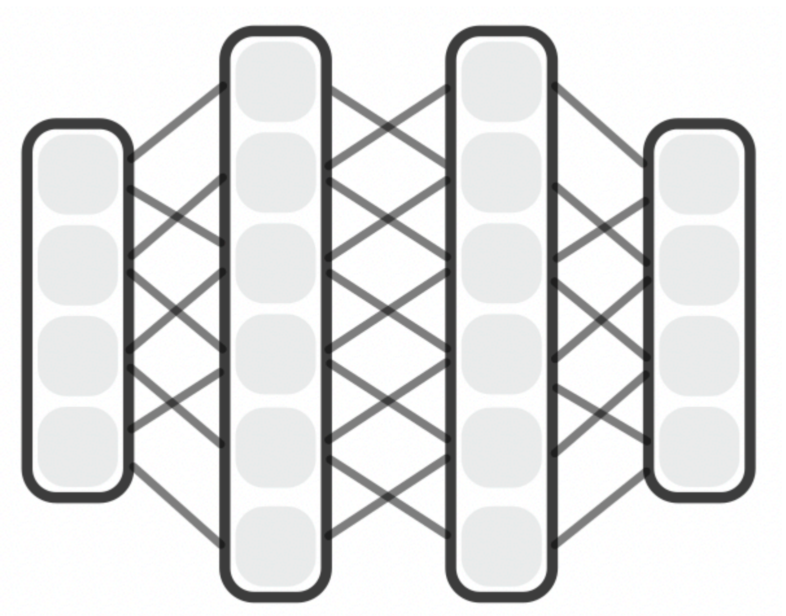
$\theta_i \sim p(\theta)$

simulated data



$\{\theta_i, x_i\}_{i=1}^{N}$

density estimator



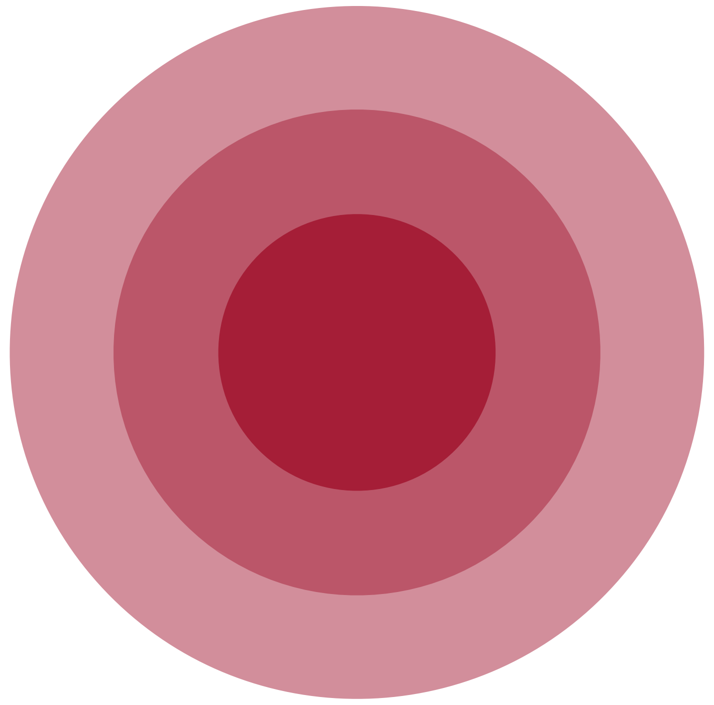
$\underset{\phi}{\text{argmin}}\ \mathcal{L}(\phi)$

- train an artificial neural network (NN) to approximate the posterior

Wood, 2010; Blum et al. 2010; Papamakarios et al. 2016, 2018

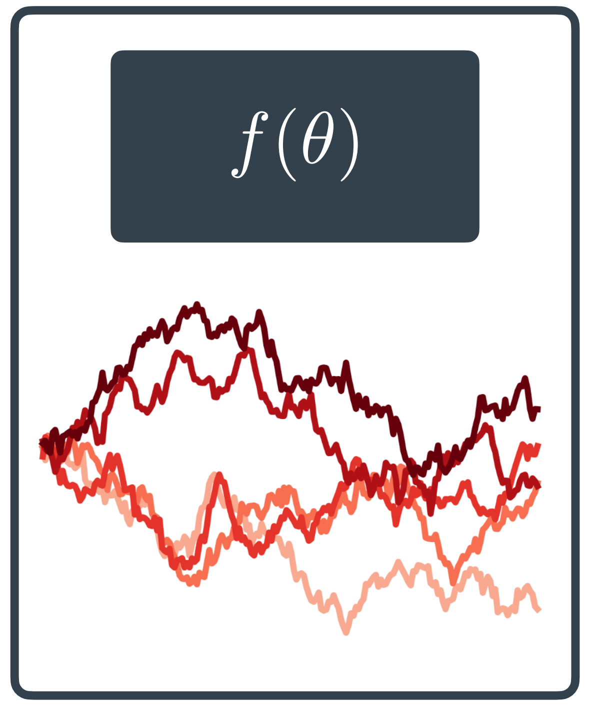
Neural Posterior Estimation (NPE)

prior



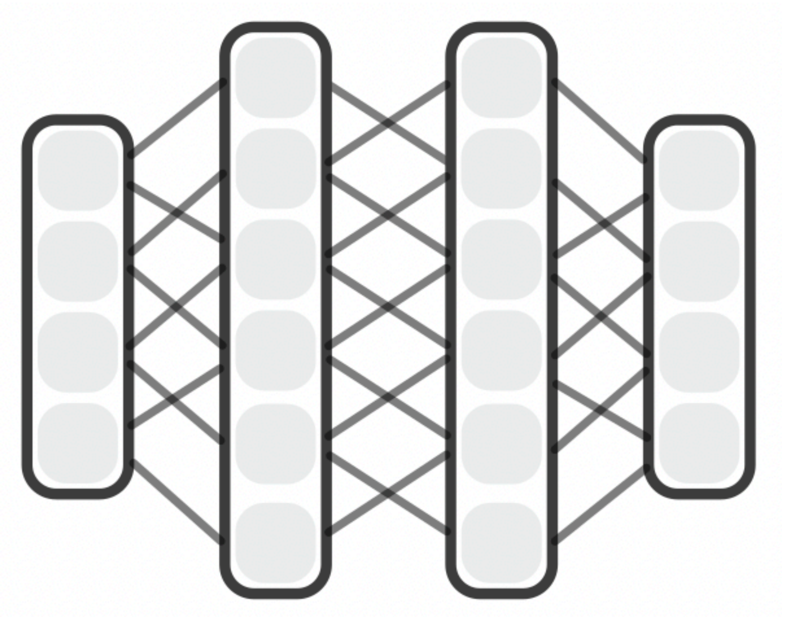
$\theta_i \sim p(\theta)$

simulated data



$\{\theta_i, x_i\}_{i=1}^{N}$

density estimator



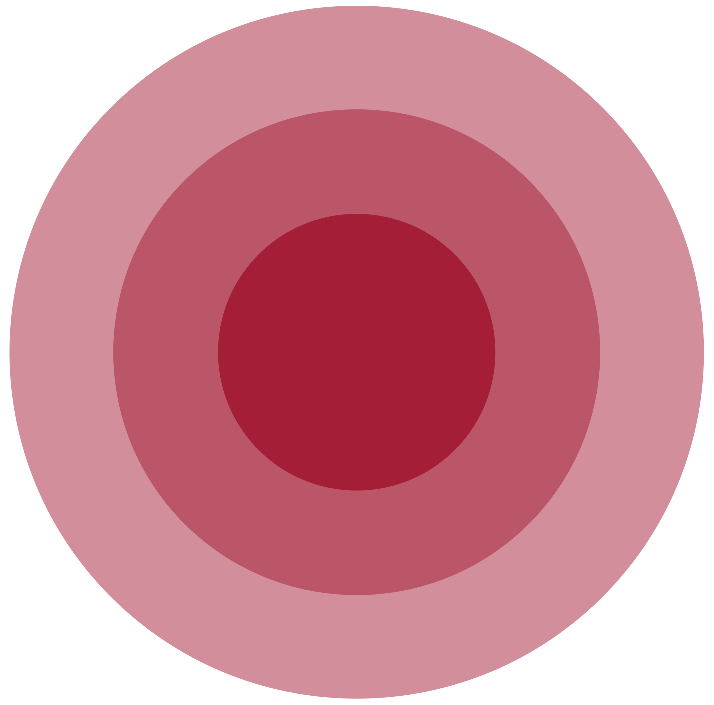
$\underset{\phi}{\text{argmin}}\ \mathcal{L}(\phi)$

- train an artificial neural network (NN) to approximate the posterior
- NN can be sampled directly

Wood, 2010; Blum et al. 2010; Papamakarios et al. 2016, 2018

Neural Posterior Estimation (NPE)

prior



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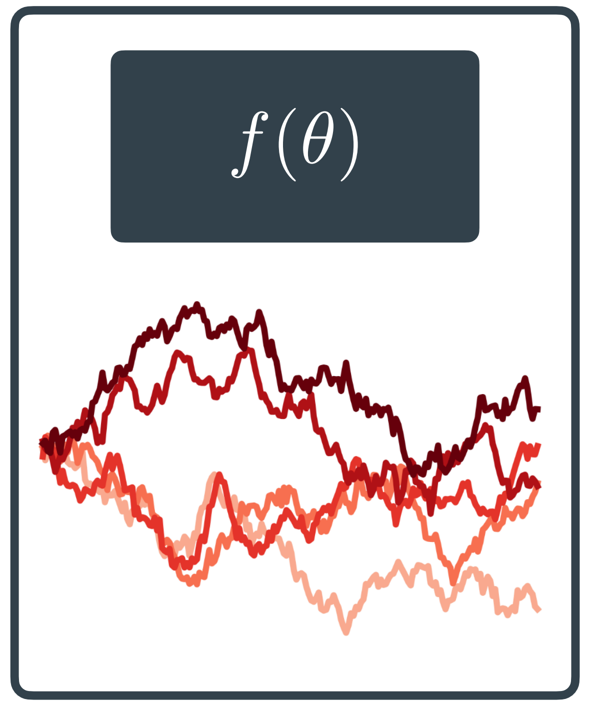

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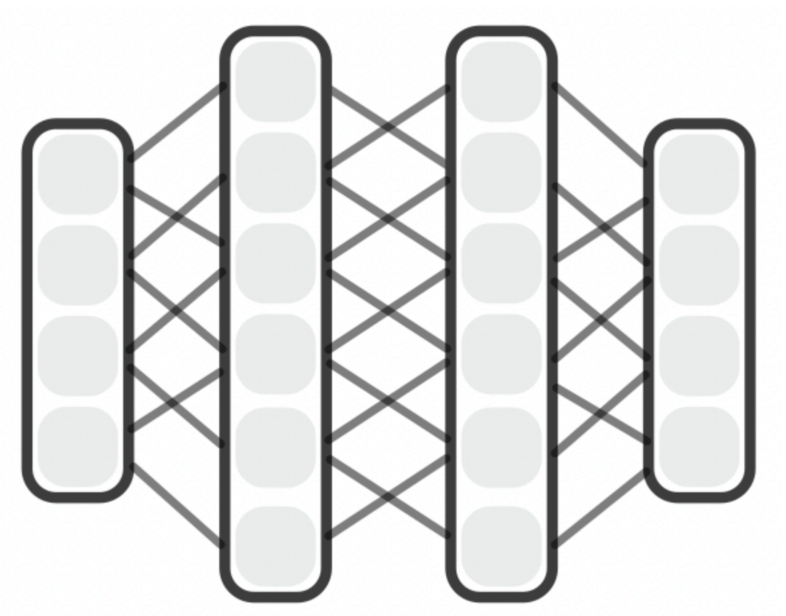
density estimator

$x_i \rightarrow$



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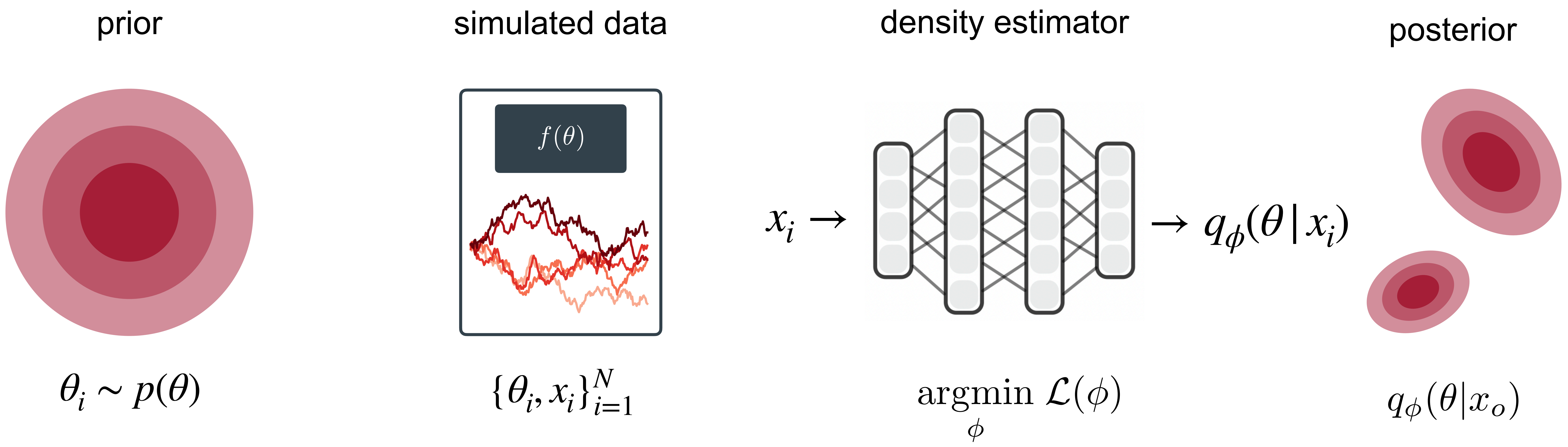

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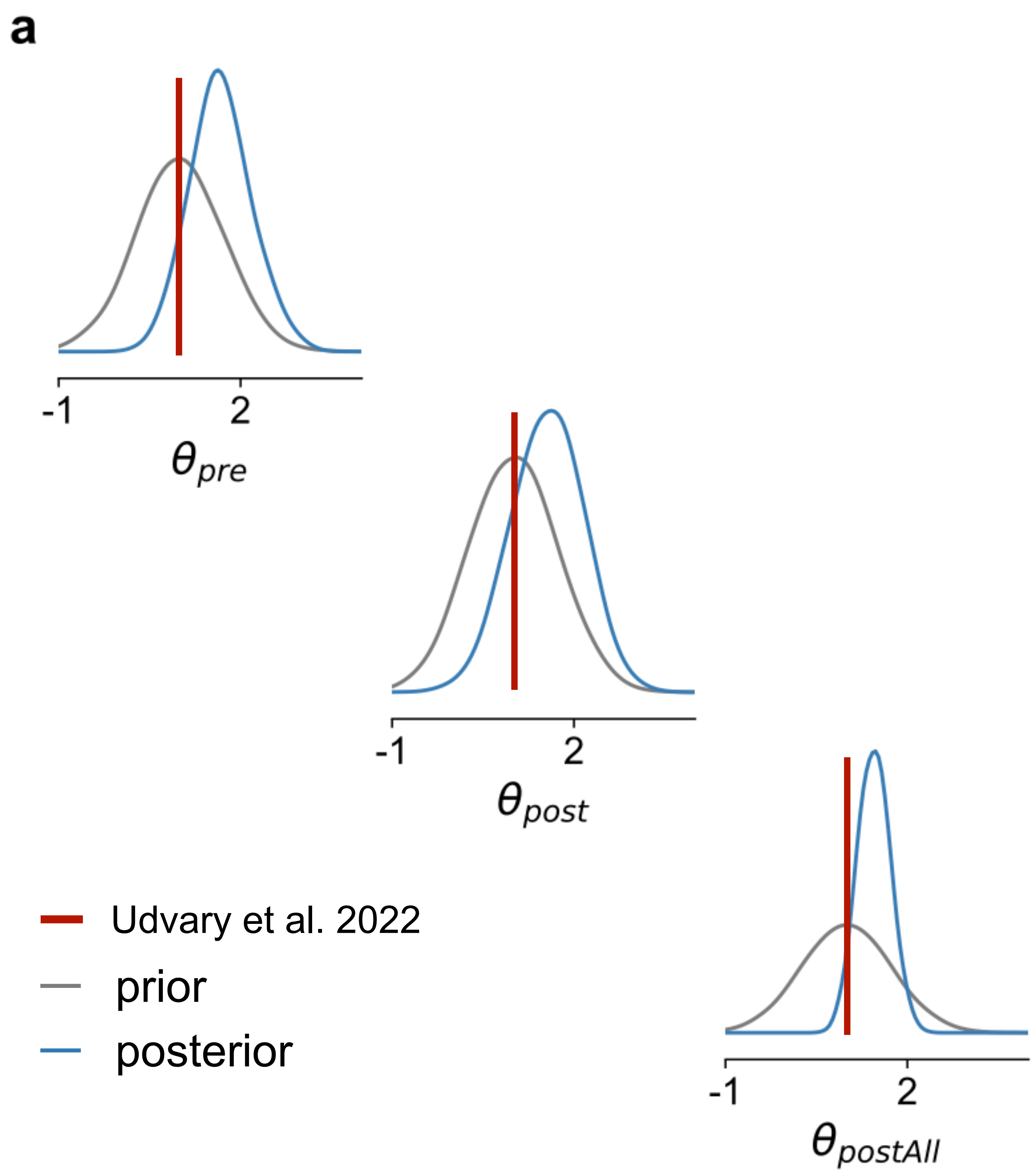
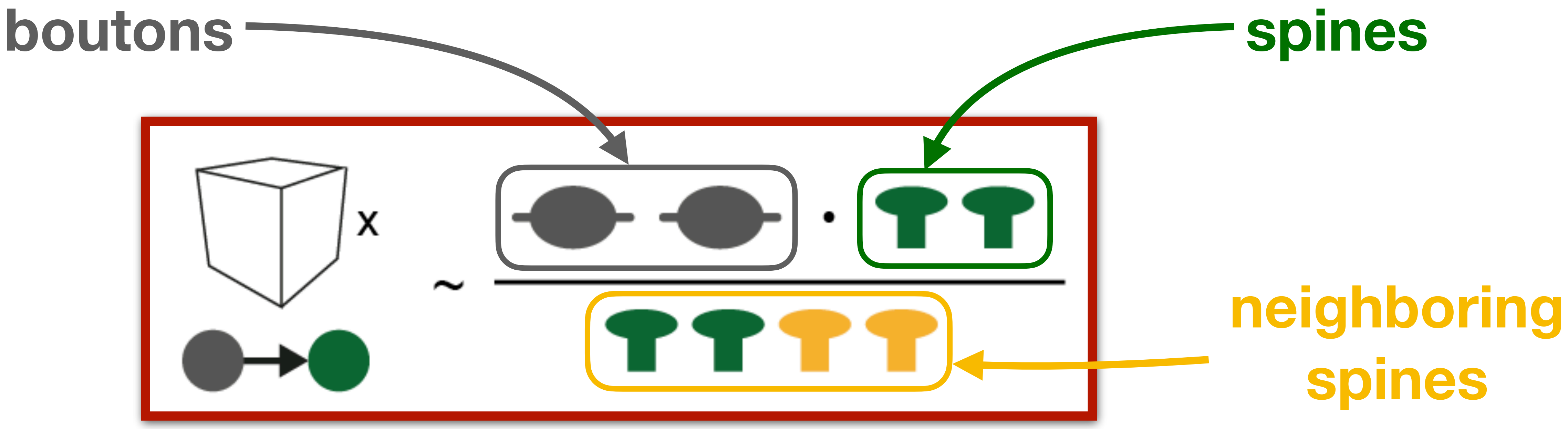
SBI identifies many possible wiring rules and reveals parameter interactions



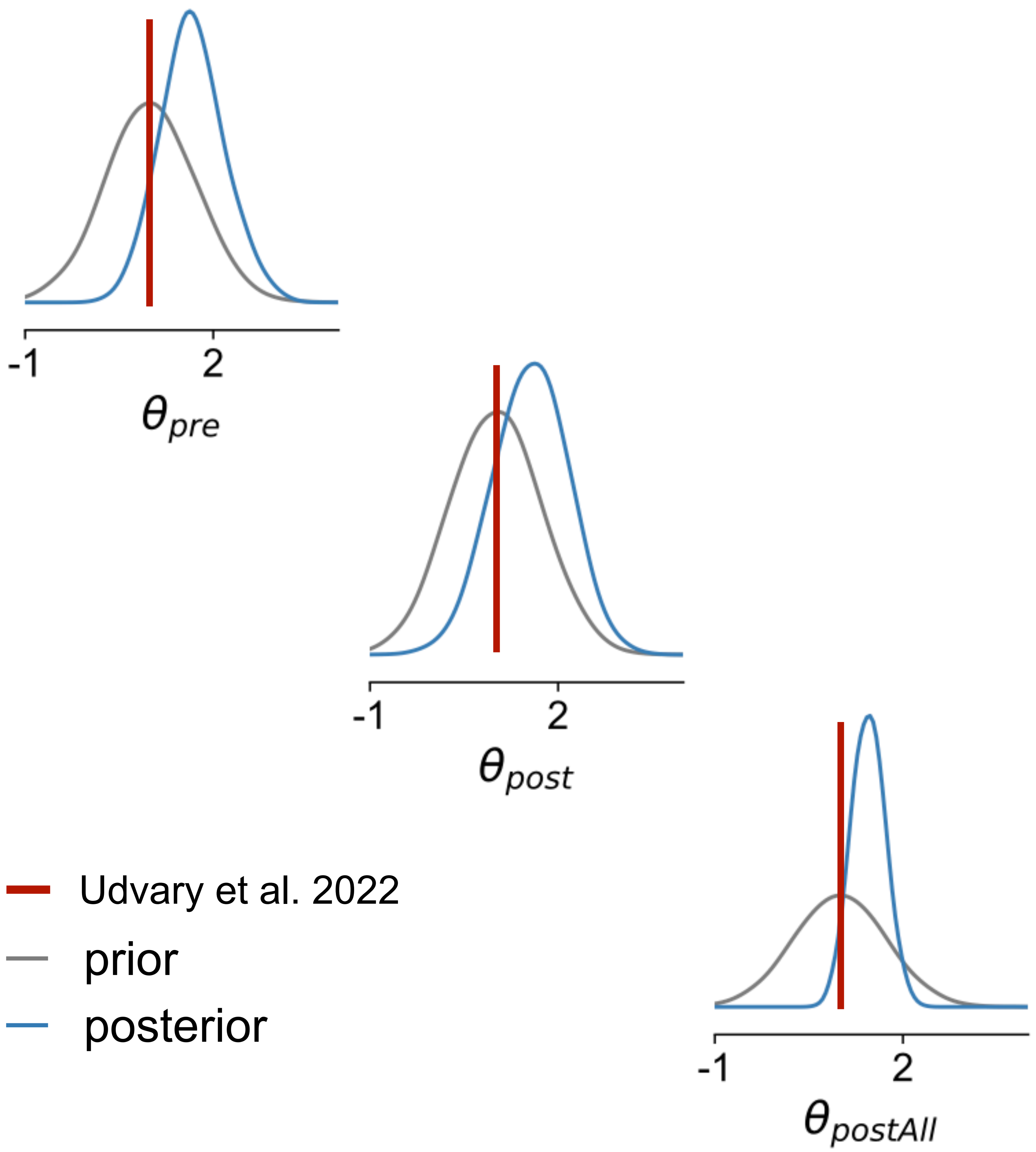


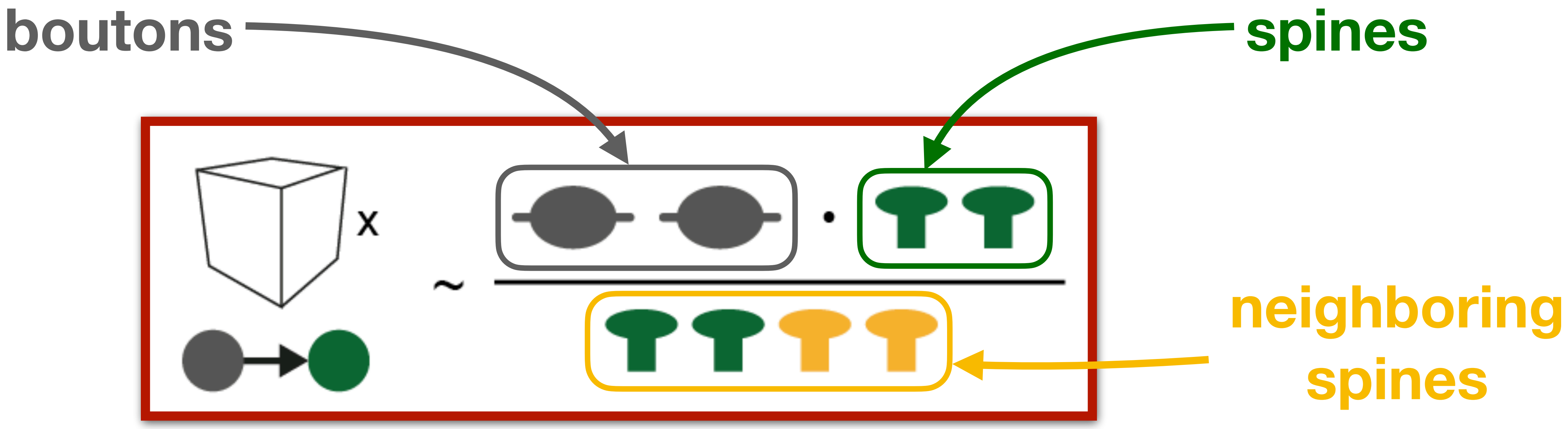
$$\mathrm{DSO}_{i,j,k}(\theta) = \frac{pre_i^{\theta_{pre}} \cdot post_j^{\theta_{post}}}{postAll_k^{\theta_{postAll}}}$$

Boelts et al. 2023

SBI identifies many possible wiring rules and reveals parameter interactions

a





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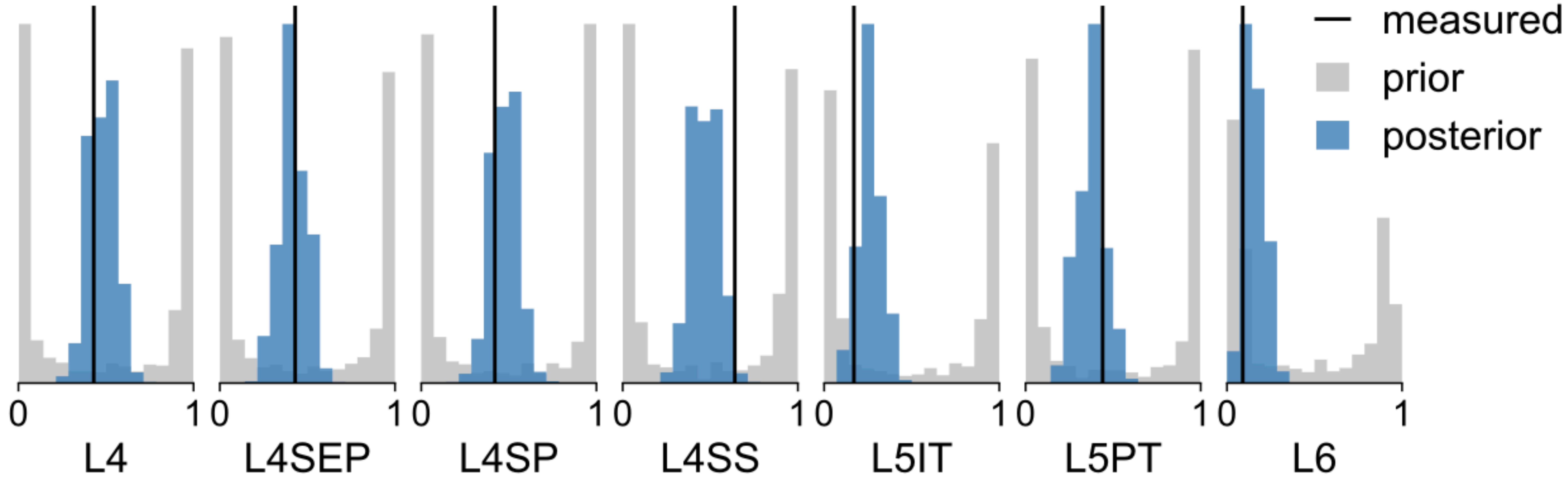

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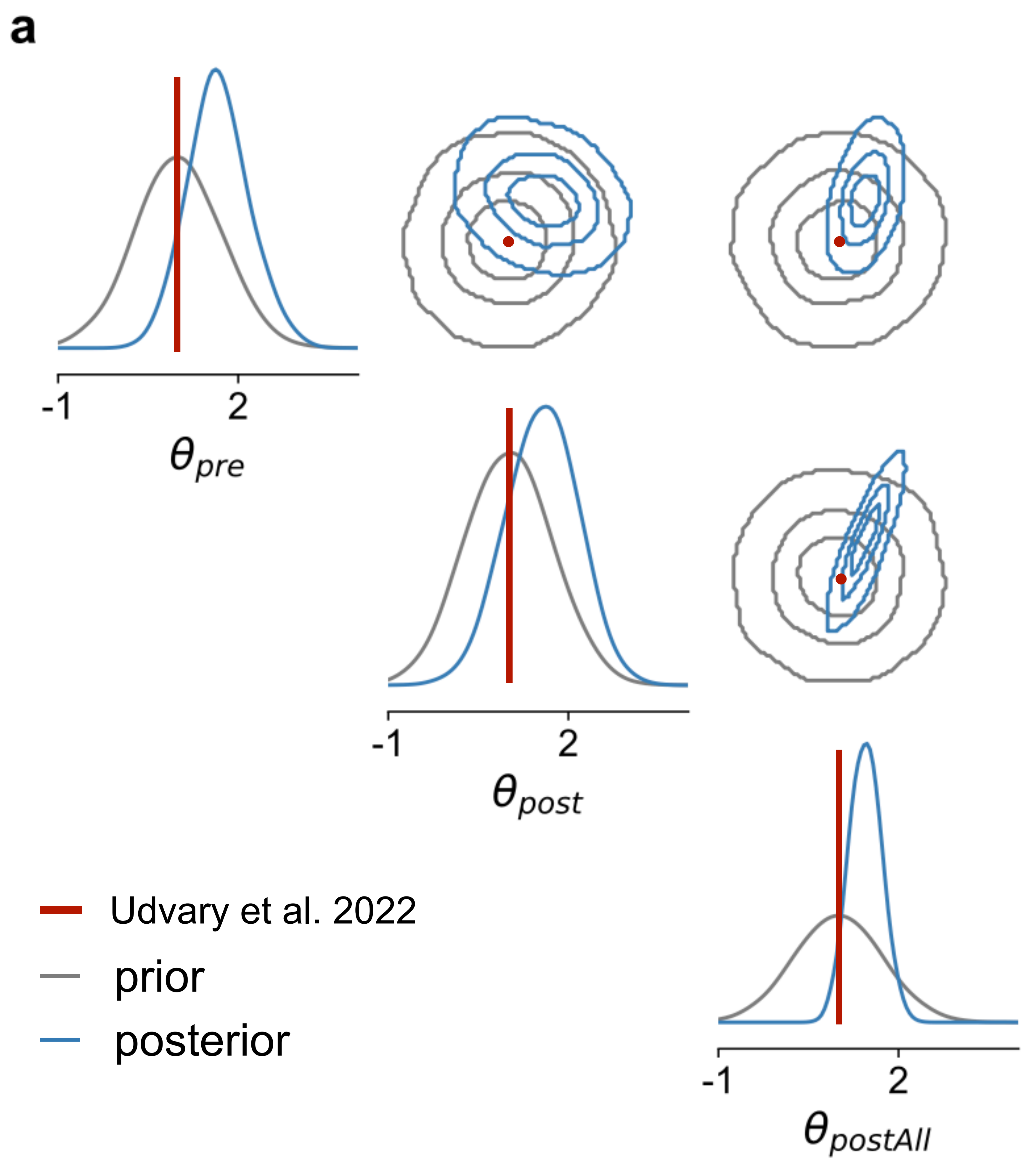

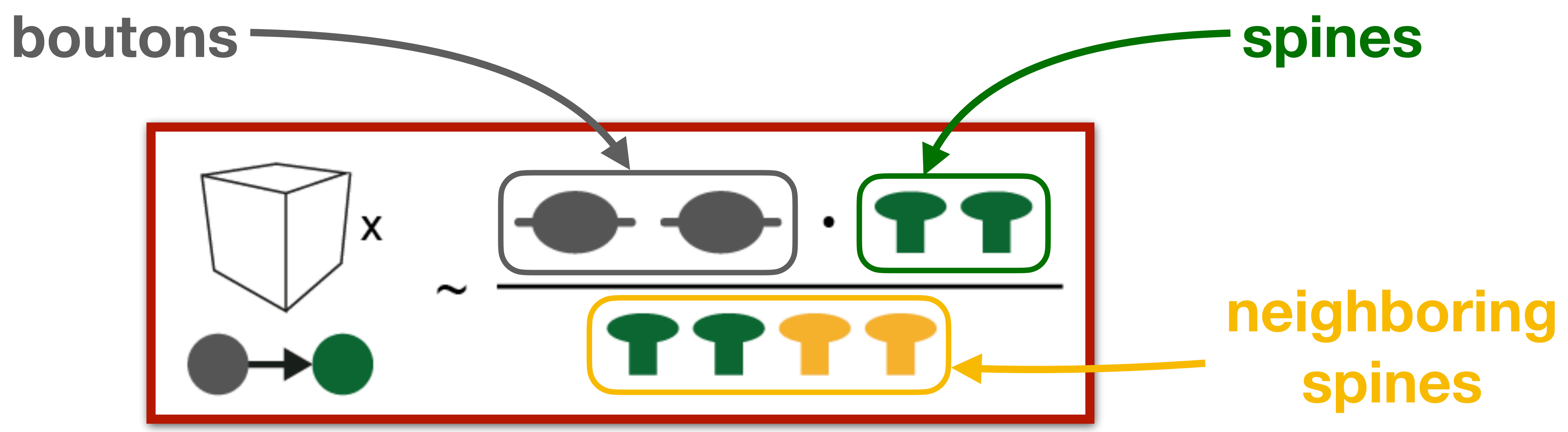

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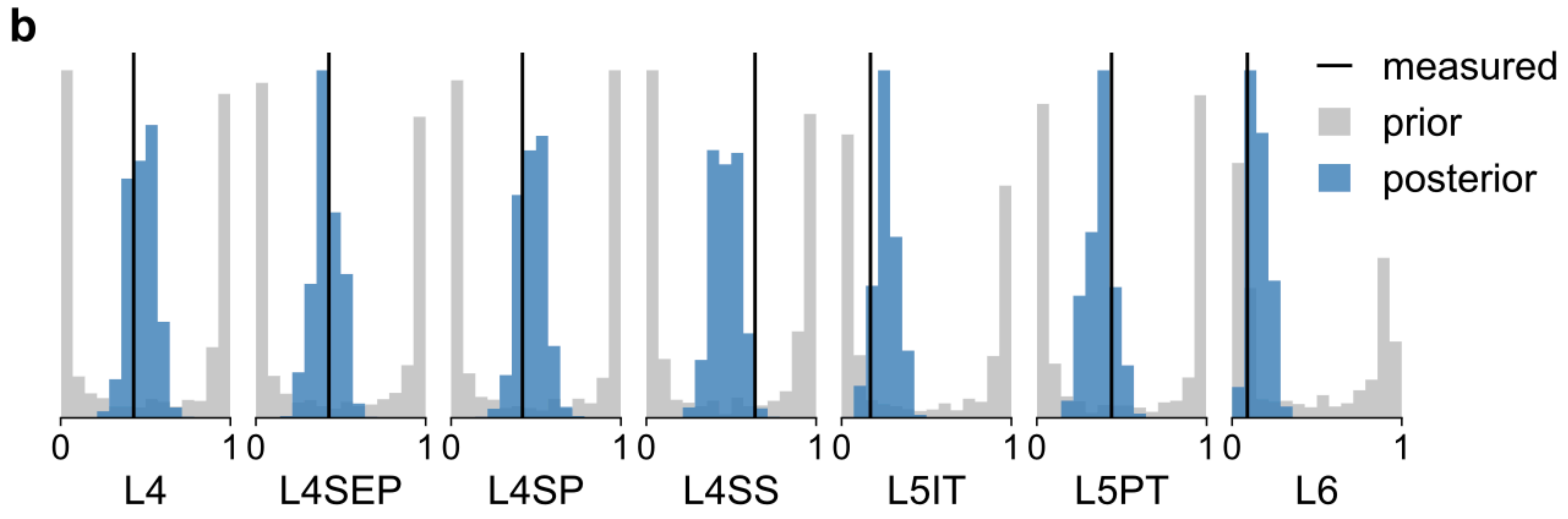
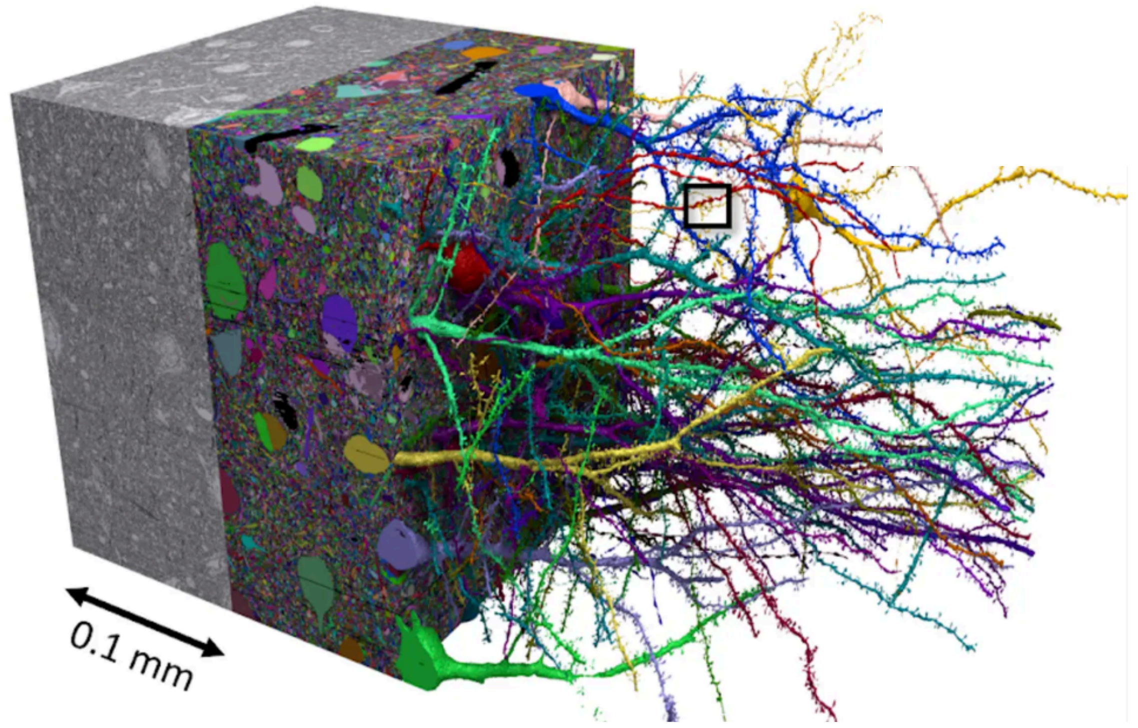


Boelts et al. 2023

Summary: SBI for connectomics

- Large amounts of data available



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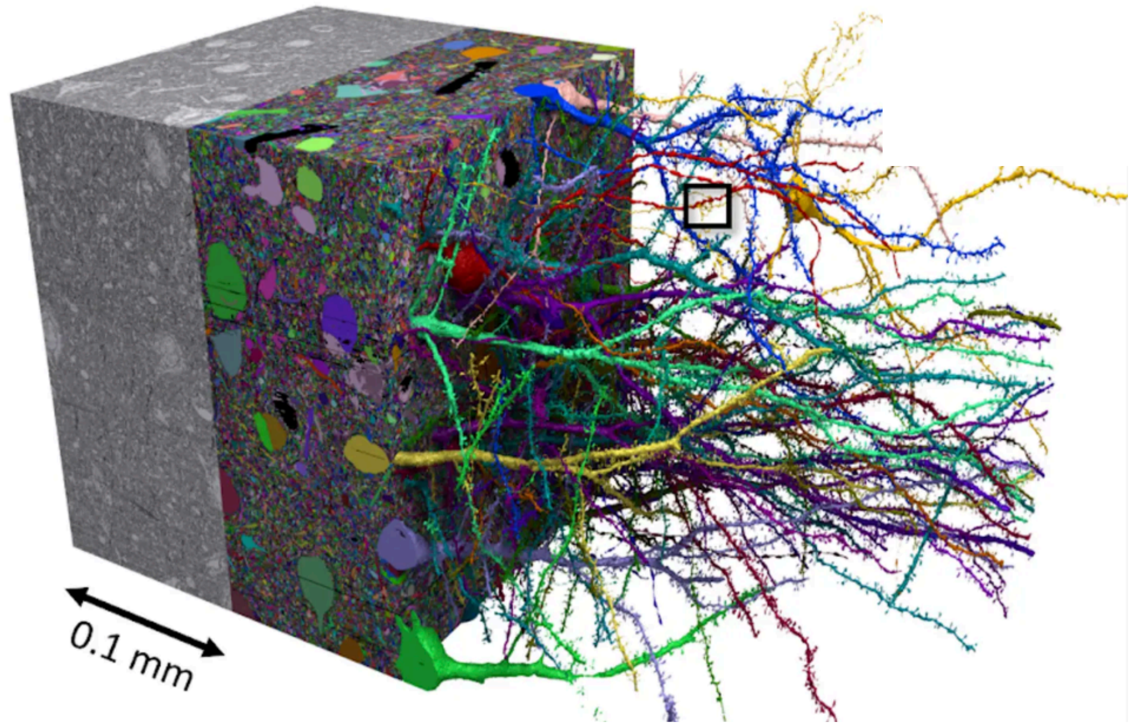

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Summary: SBI for connectomics

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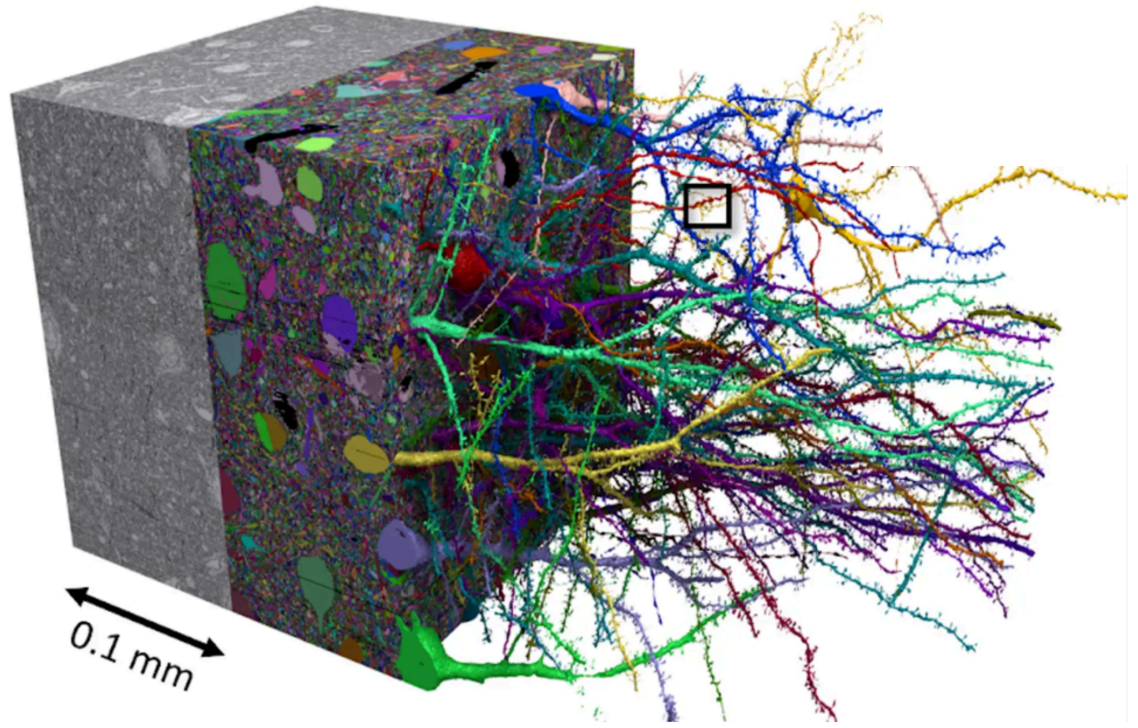
- Use parametrized wiring rules to test hypotheses
- SBI enables us to constrain and interpret the parameters efficiently



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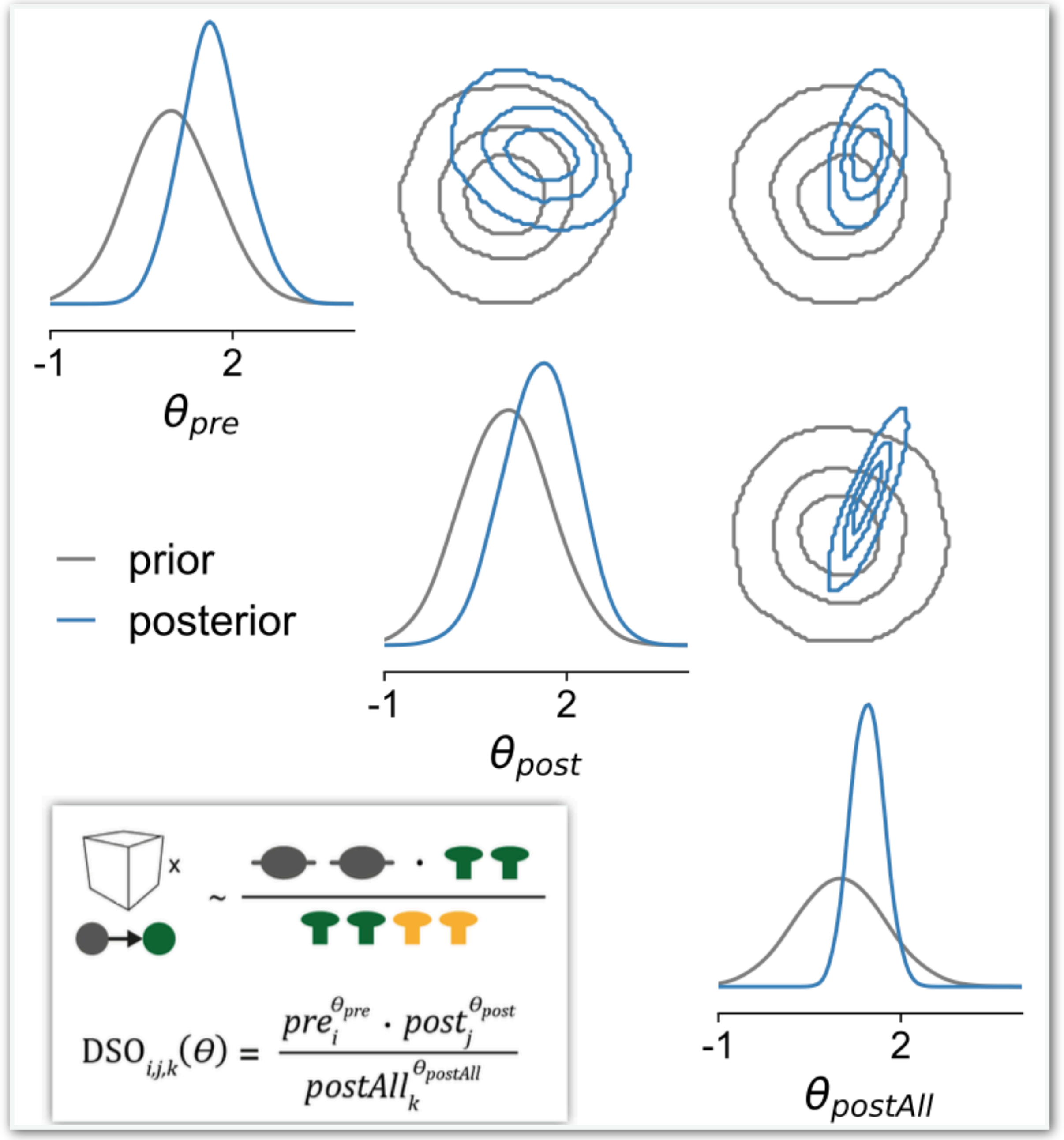
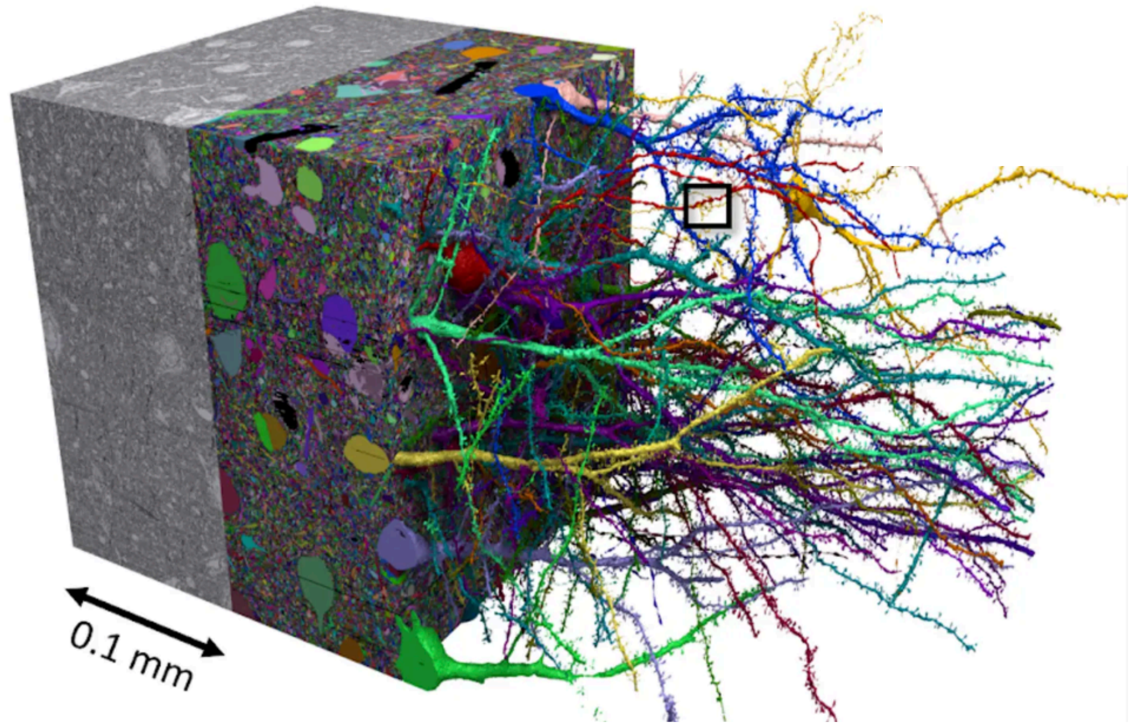


Summary: SBI for connectomics

- Large amounts of data available
- Use parametrized wiring rules to test hypotheses
- SBI enables us to constrain and interpret the parameters efficiently
- Faster and more flexible exploration of hypotheses



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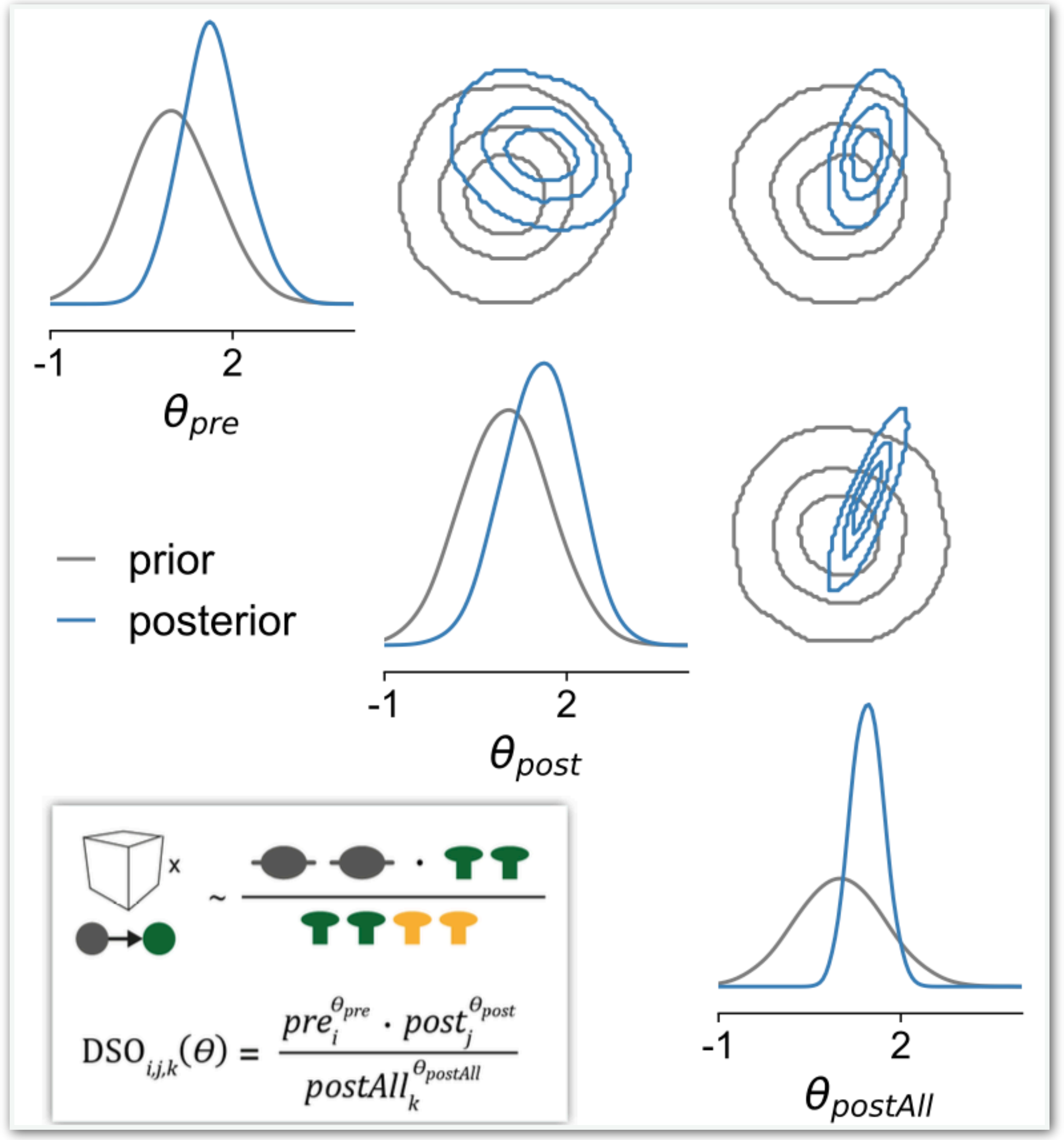

Advancing Methods and Applicability of SBI in neuroscience

1. A new SBI method for **decision-making research** ✓
2. How to apply SBI in **Connectomics** ✓
3. Software tools and guidelines for SBI

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SNLE, SNPE, SNRE

diffusion models

flow matching

Tejero-Cantero, **Boelts****, *Deistler*, Lueckmann*, Durkan* et al. 2020*

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- Which method to use?
- How to use it?
- Is there usable code?
- How does it compare to other methods
- …

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JOSS
The Journal of Open Source Software

sbi: A toolkit for simulation-based inference

Alvaro Tejero-Cantero[e, 1], Jan Boelts[e, 1], Michael Deistler[e, 1], Jan-Matthis Lueckmann[e, 1], Conor Durkan[e, 2], Pedro J. Gonçalves[1, 3], David S. Greenberg[1, 4], and Jakob H. Macke[1, 5, 6]

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An accessible toolkit for applying SBI

sbi

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Installation
Tutorials and Examples
Contributing
API Reference
FAQ
Credits

sbi : simulation-based inference

sbi : A Python toolbox for simulation-based inference.

```
prior = BoxUniform(low=zeros(2), high=2*ones(2))   # Box prior [0,2]x[0,2]
def simulator(θ): return θ + 0.1*randn_like(θ)     # Gaussian in 2D
```

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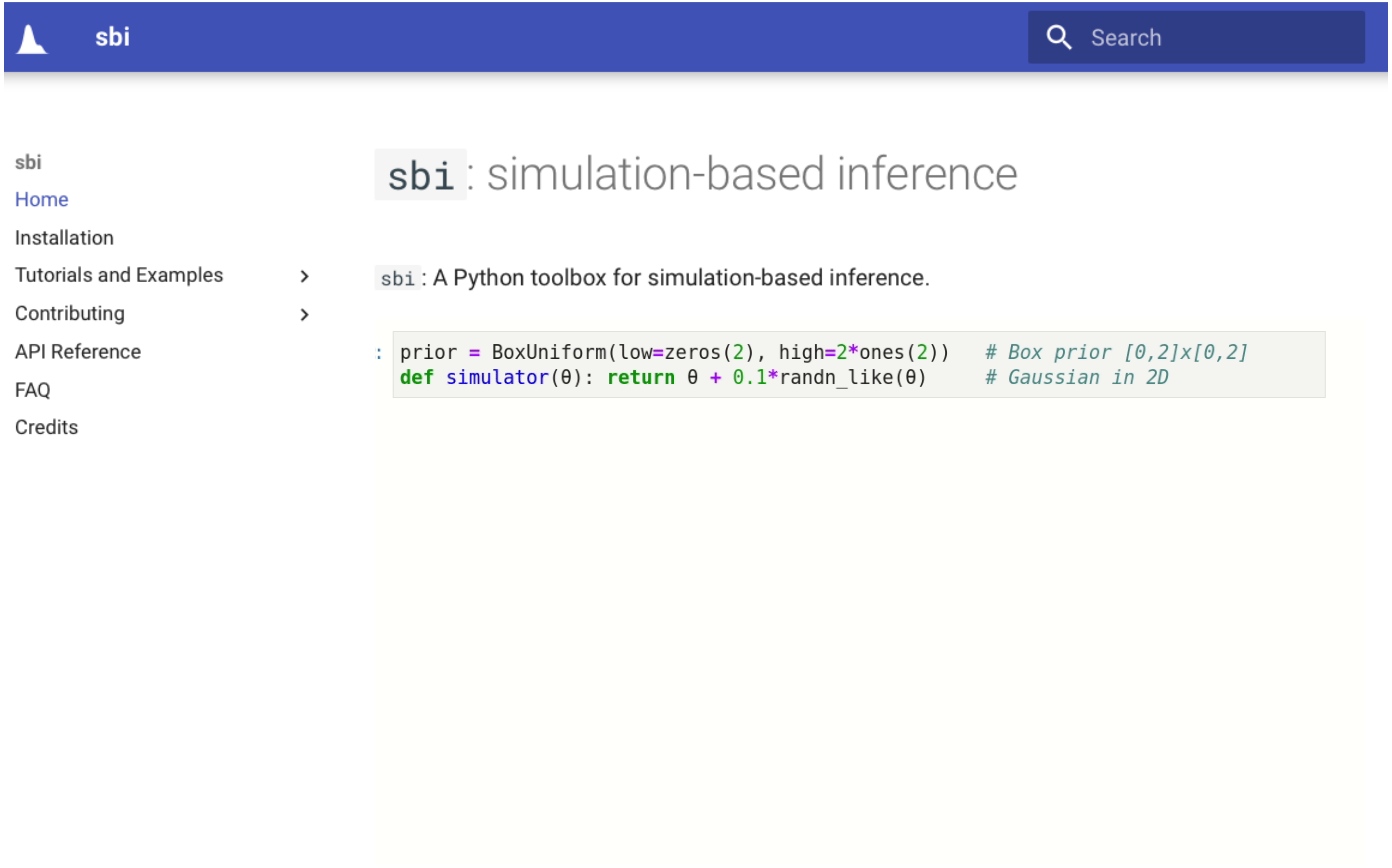

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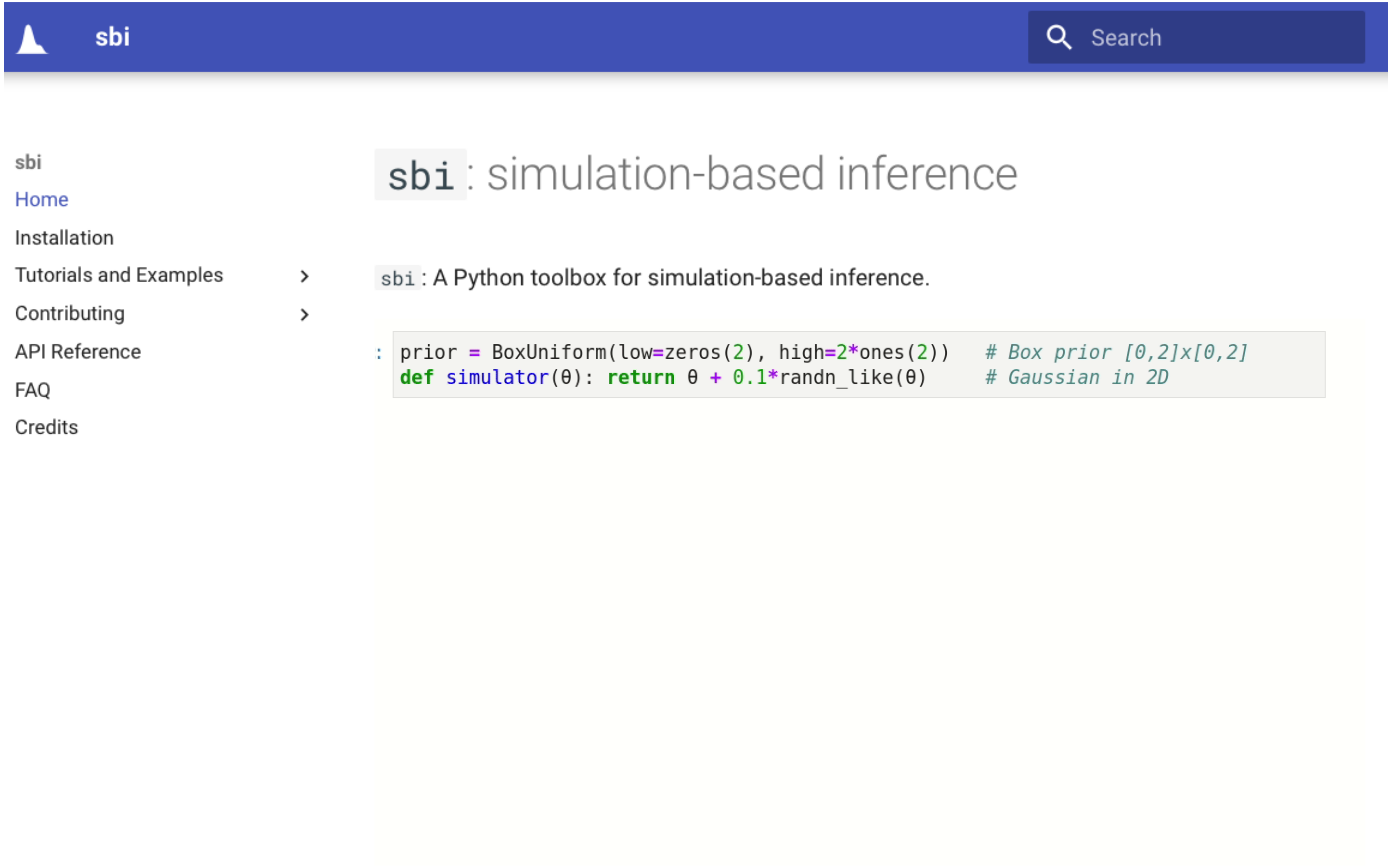

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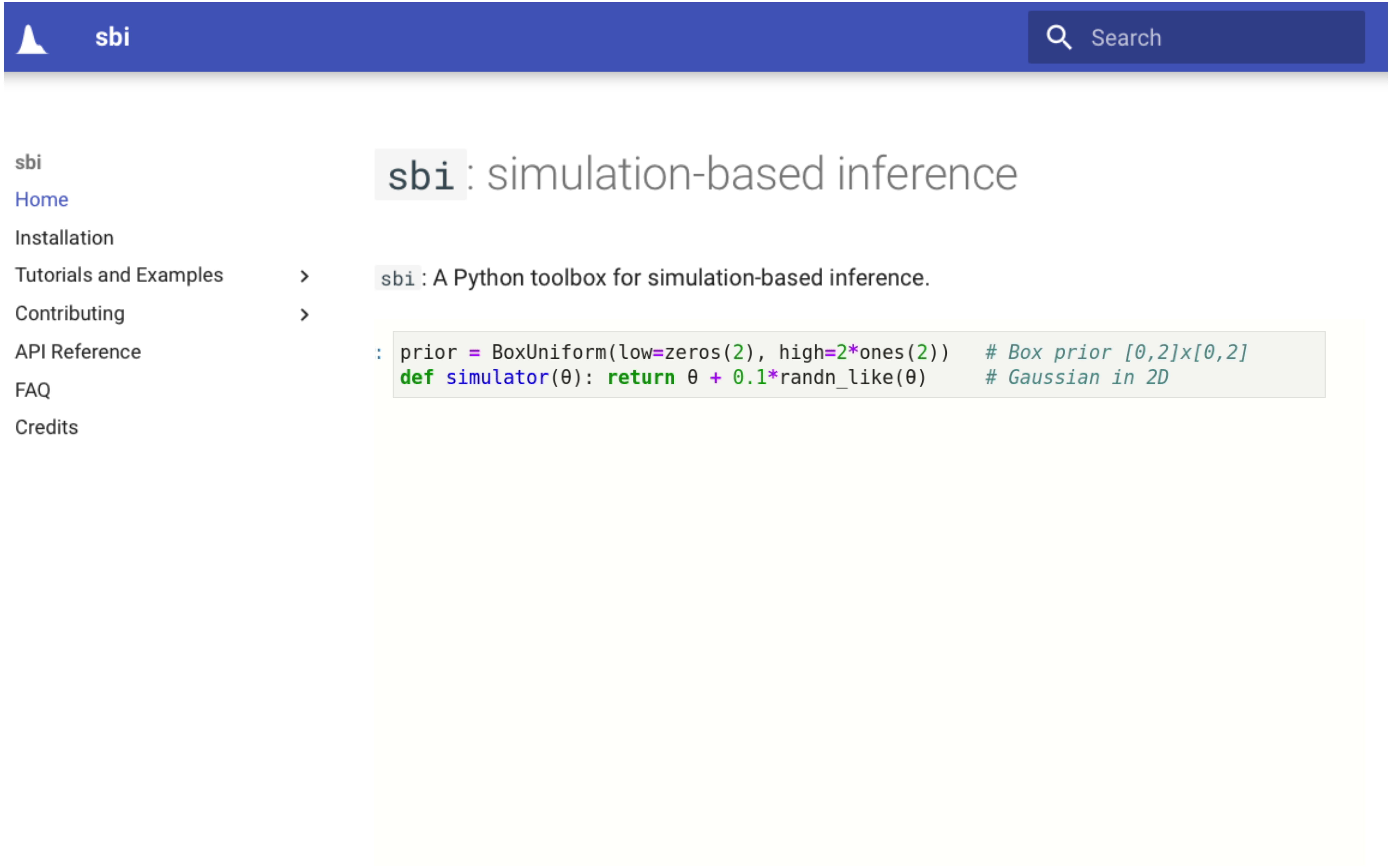

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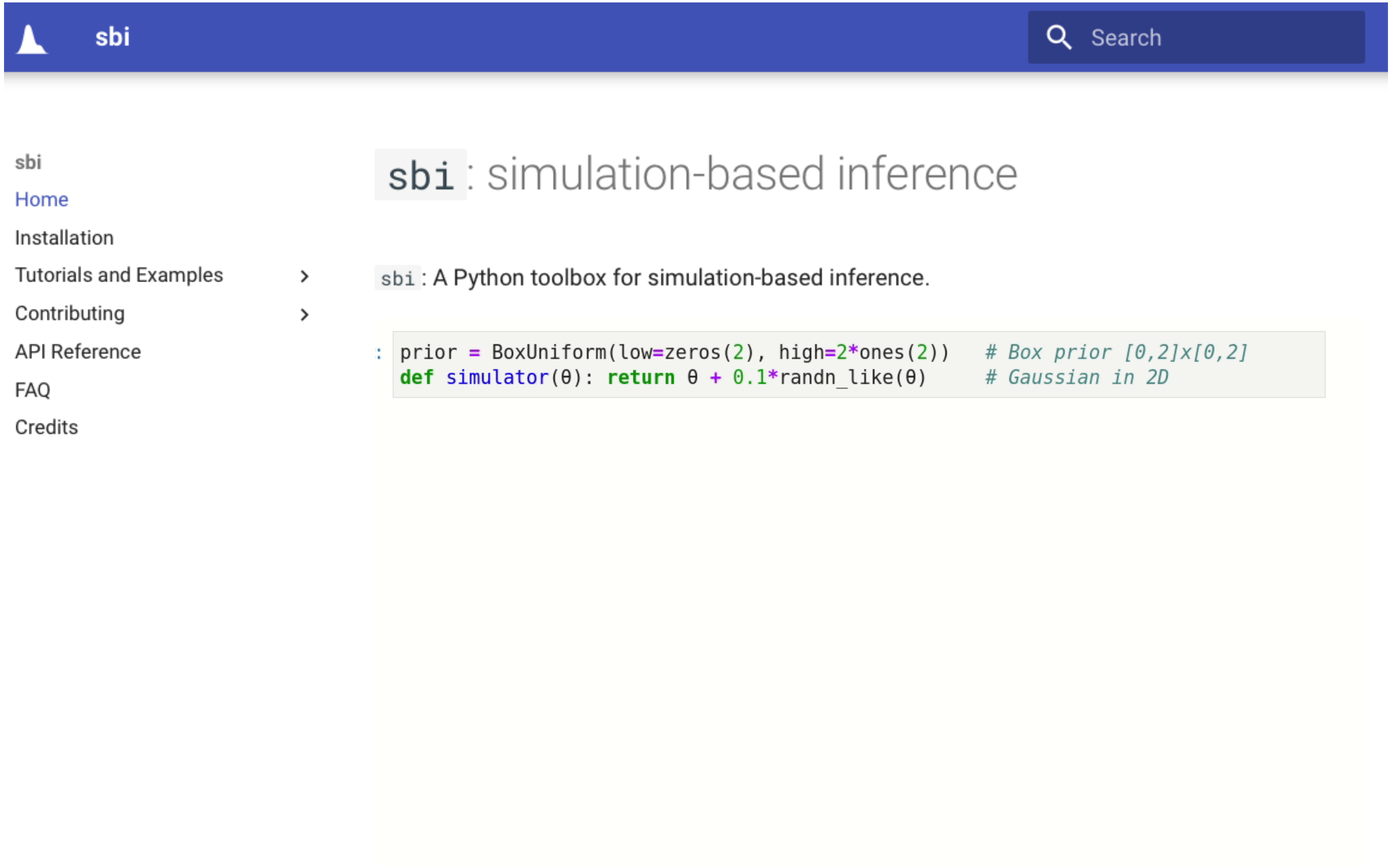

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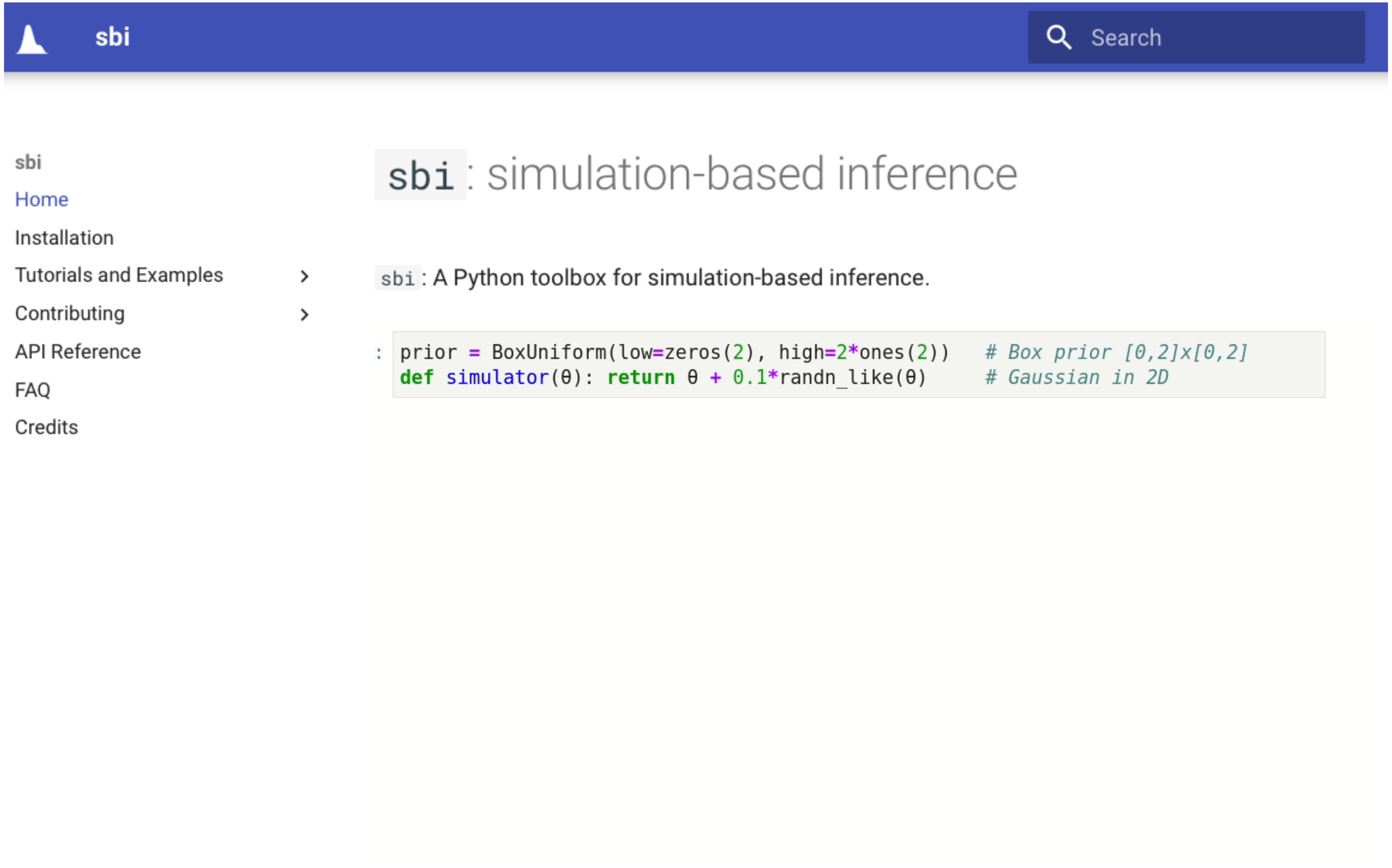

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PNAS RESEARCH ARTICLE | NEUROSCIENCE

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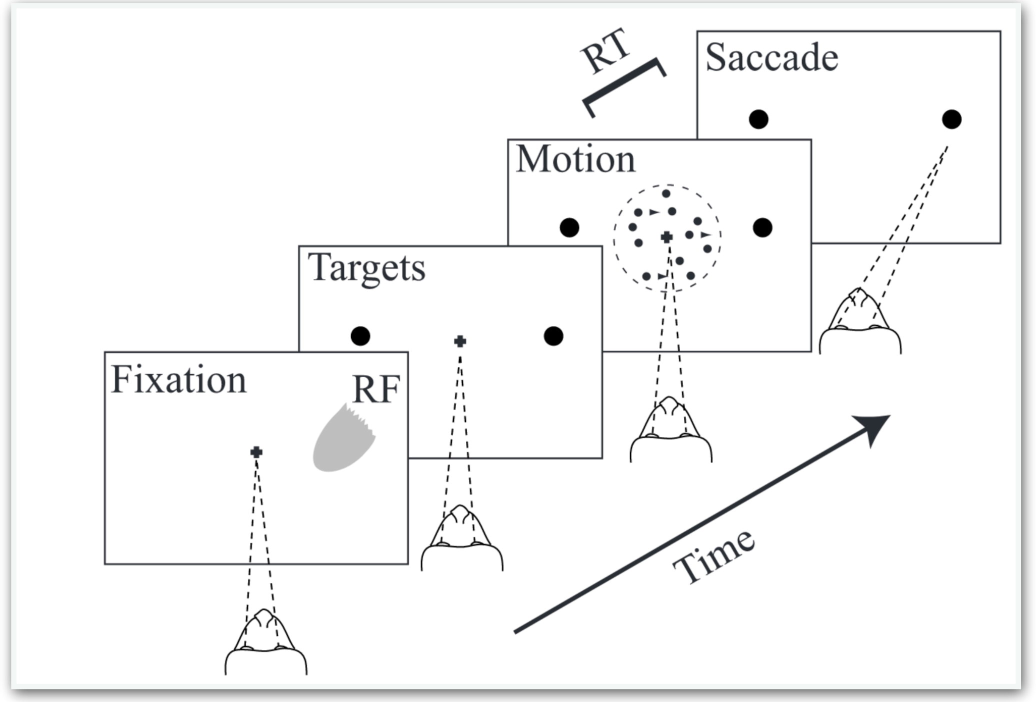
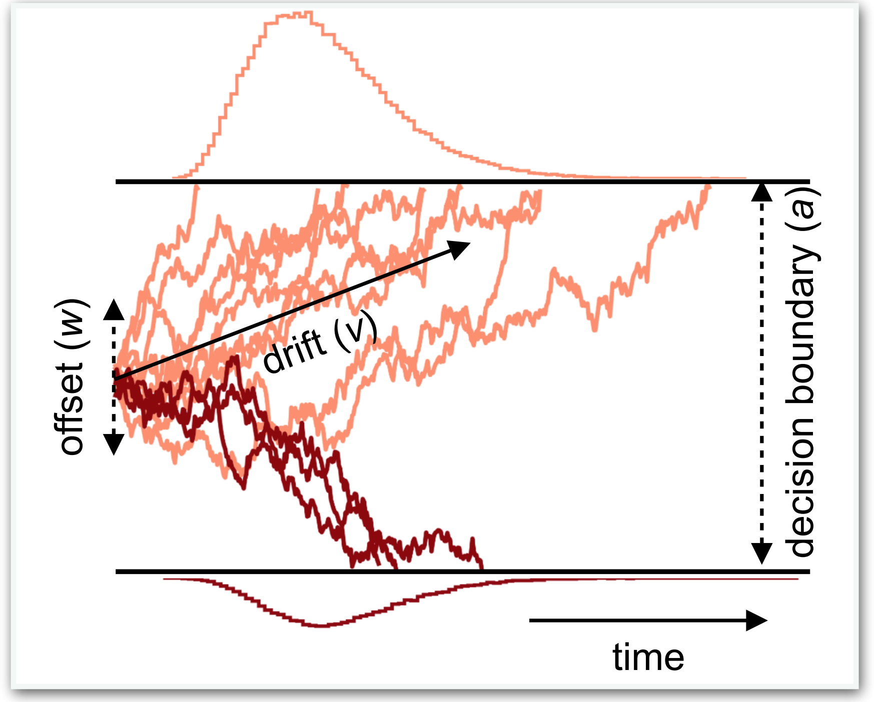
   - Inference for custom models of decision-making





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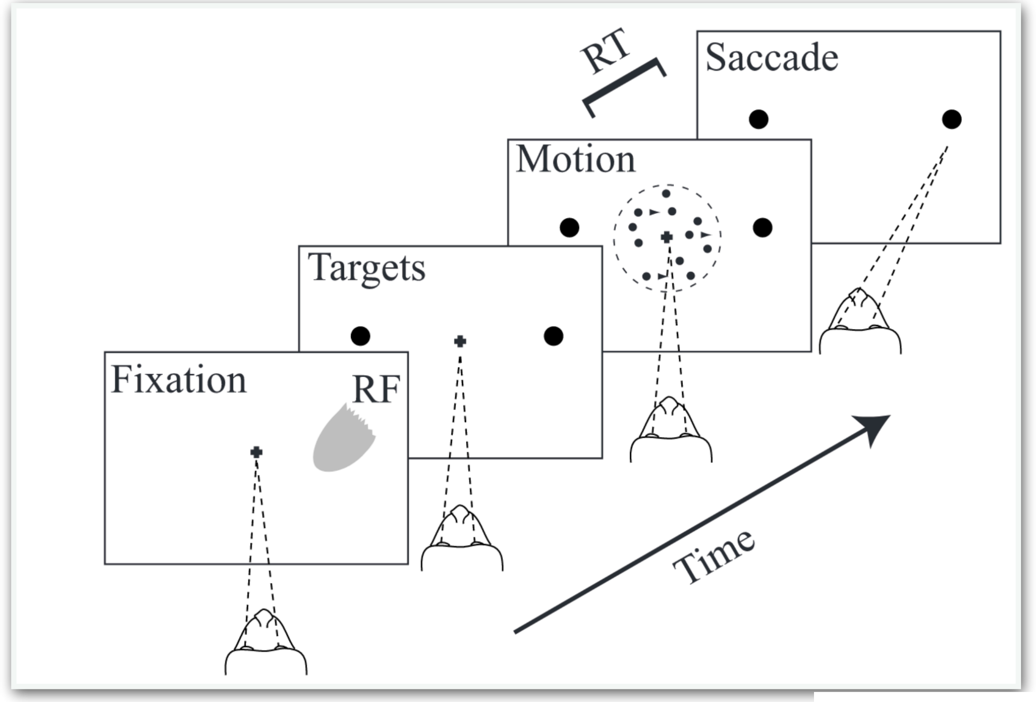

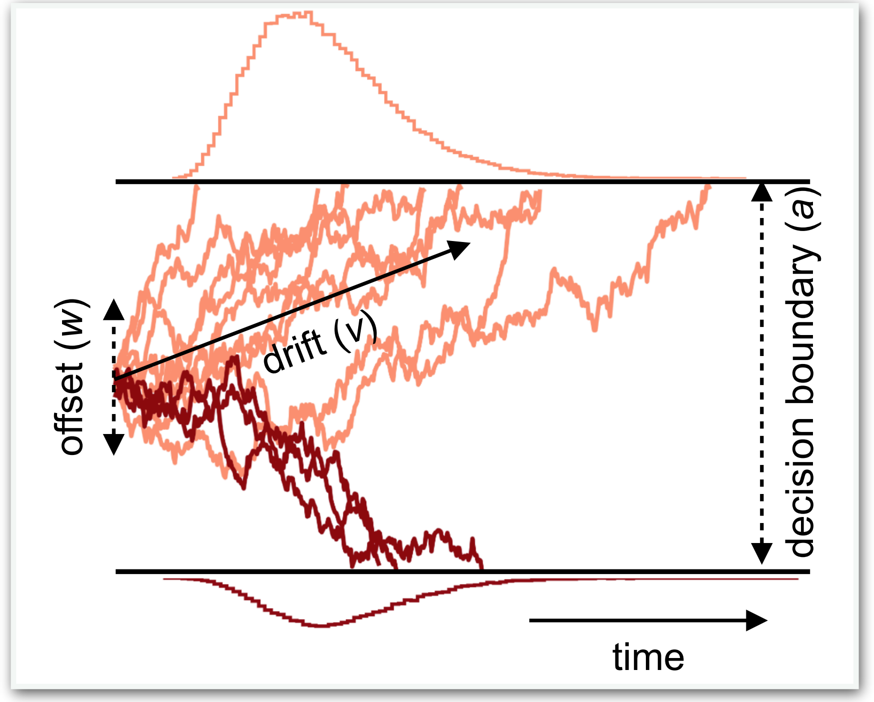

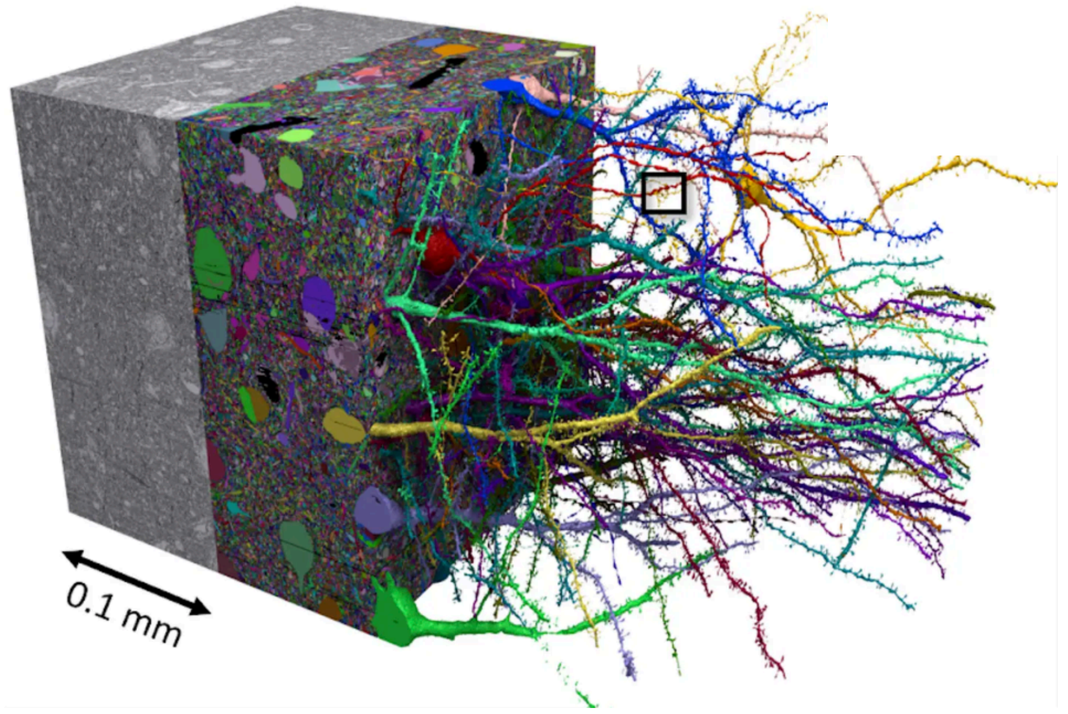

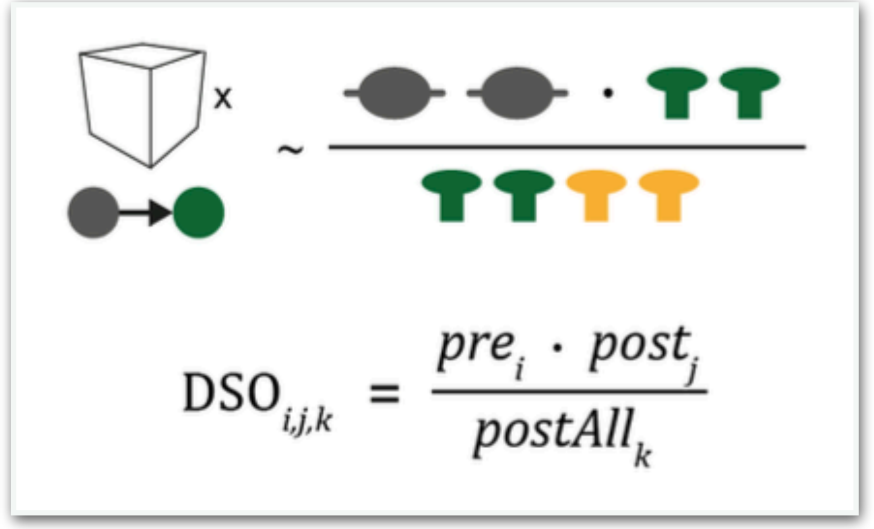

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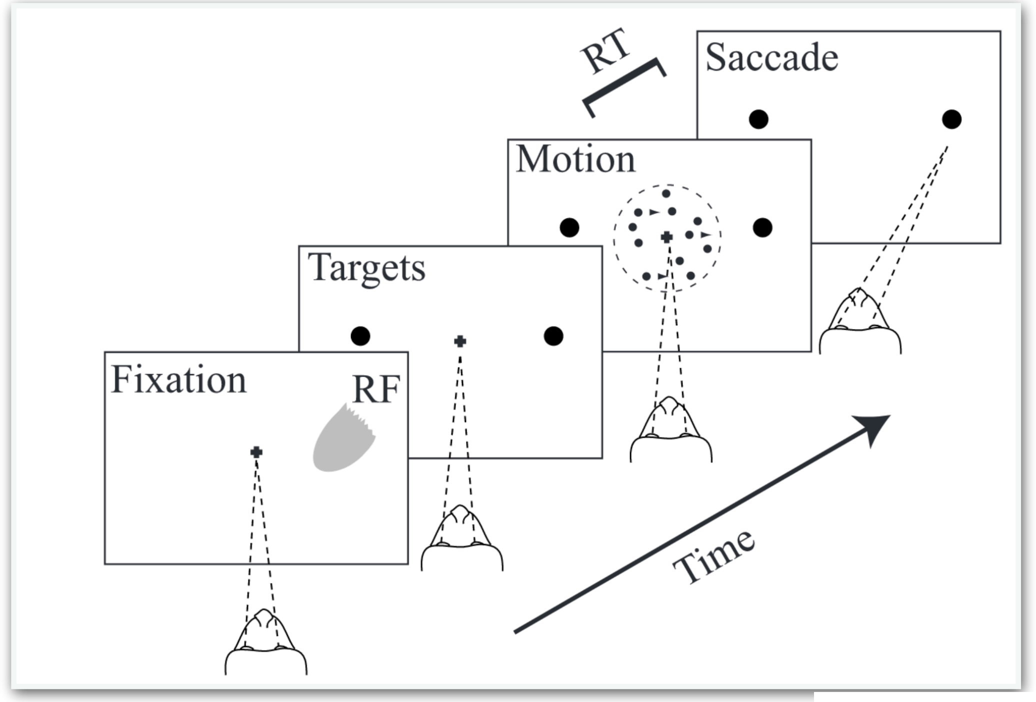

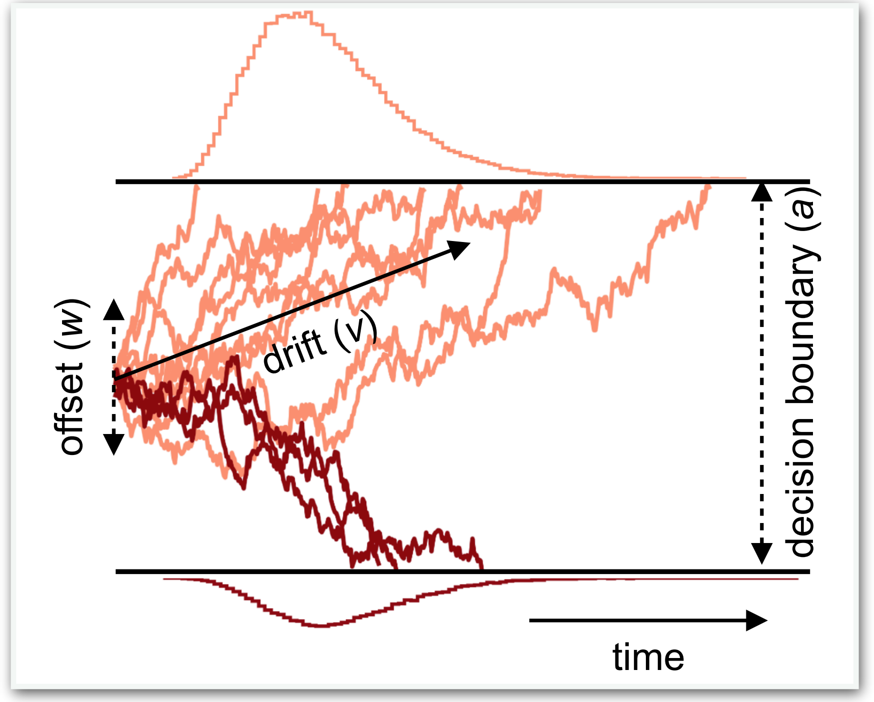

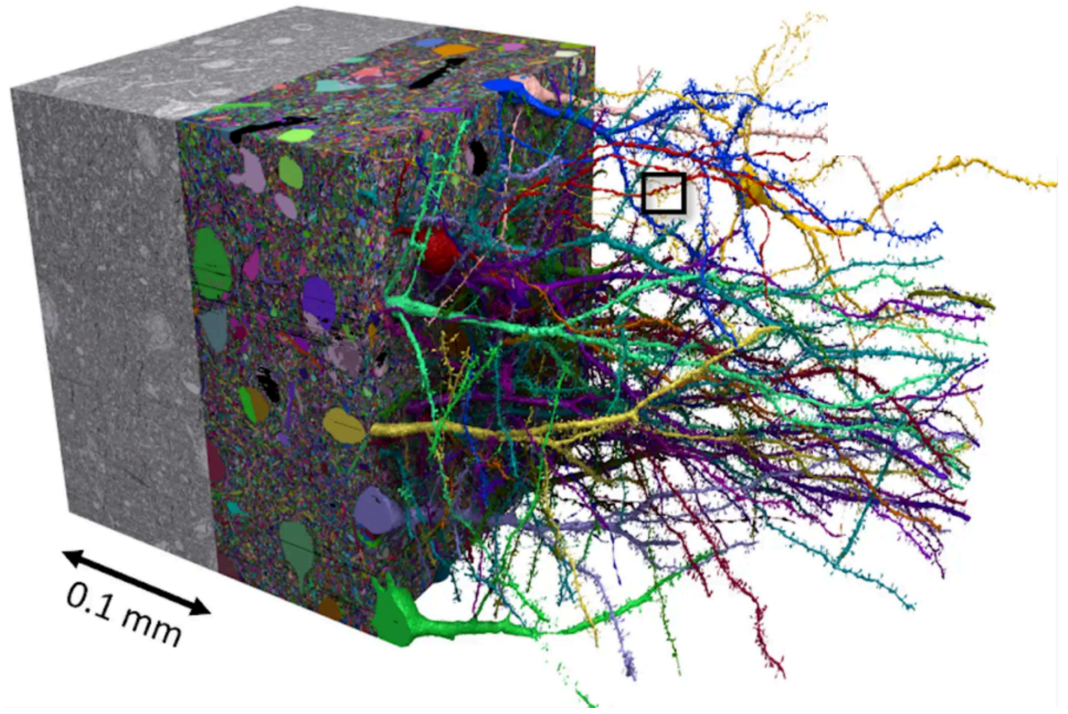

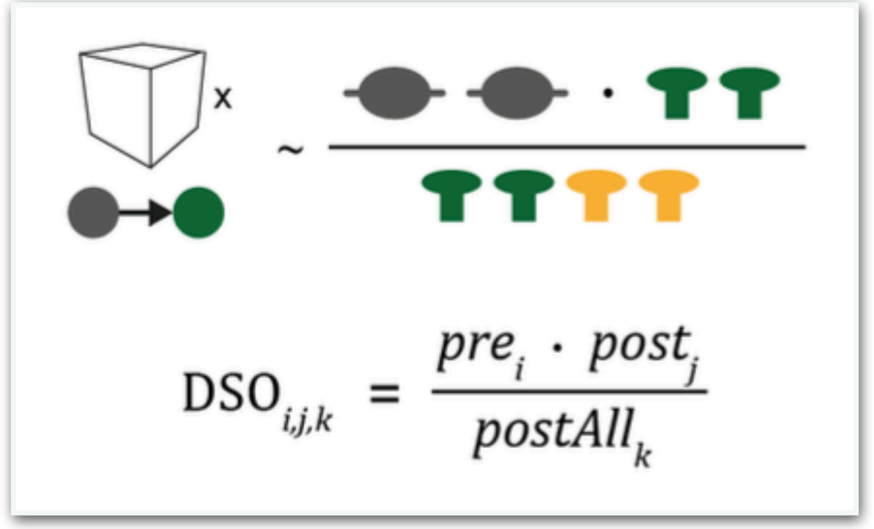

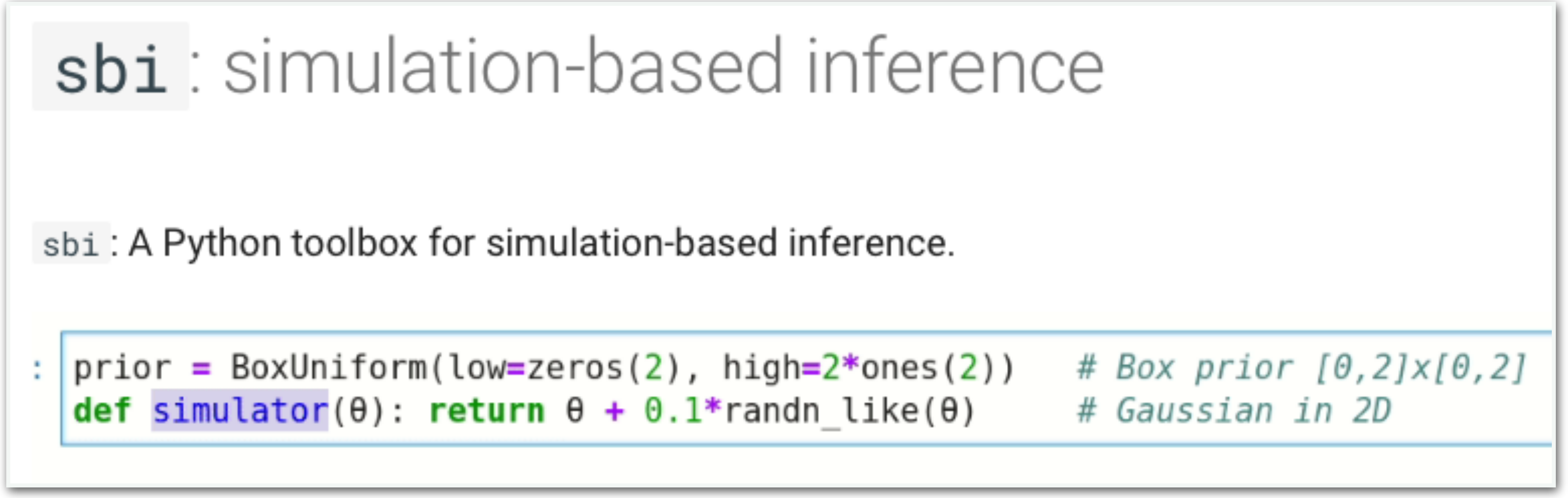

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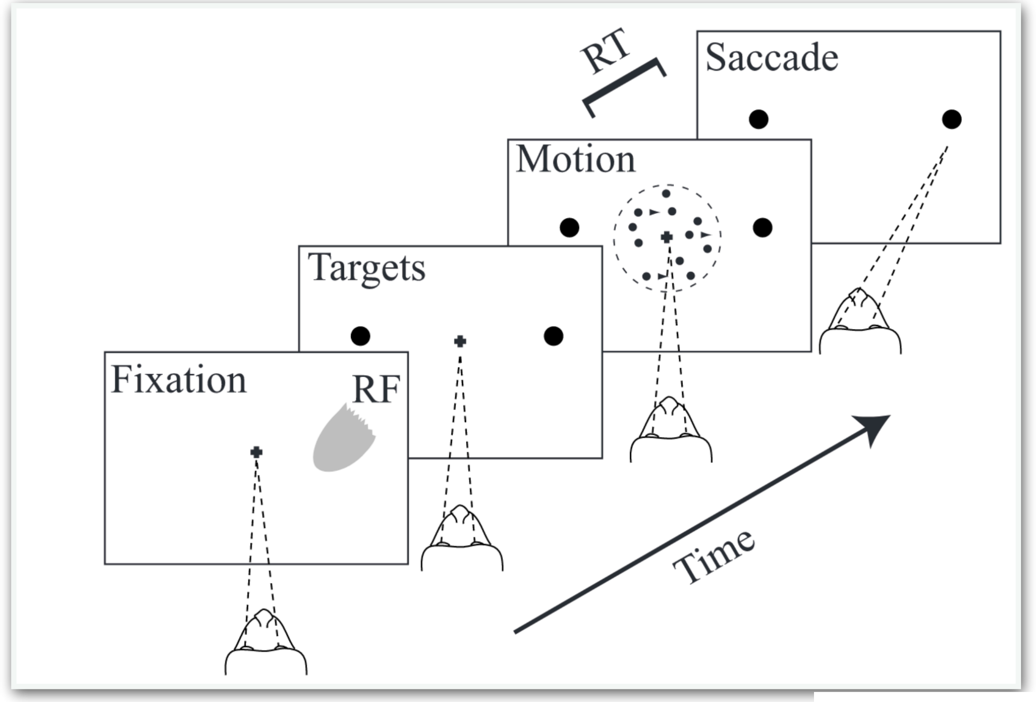
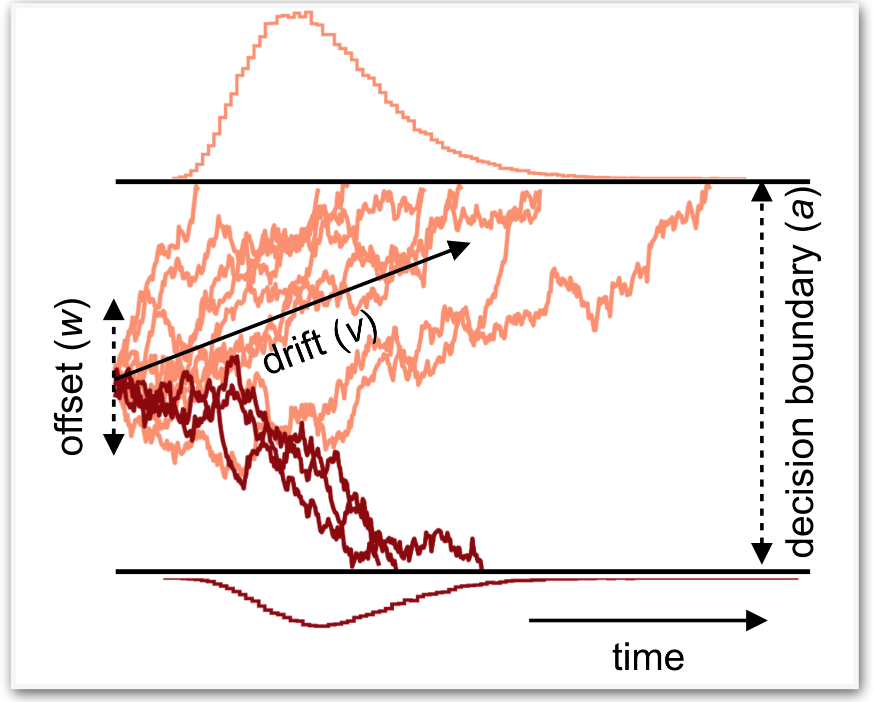
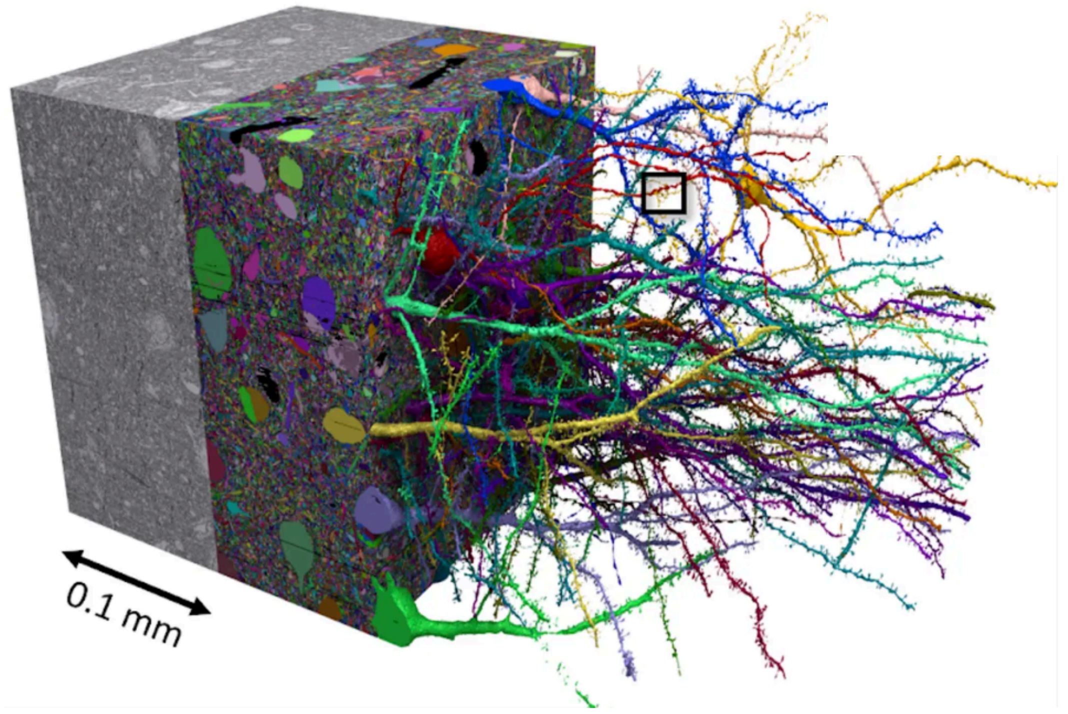
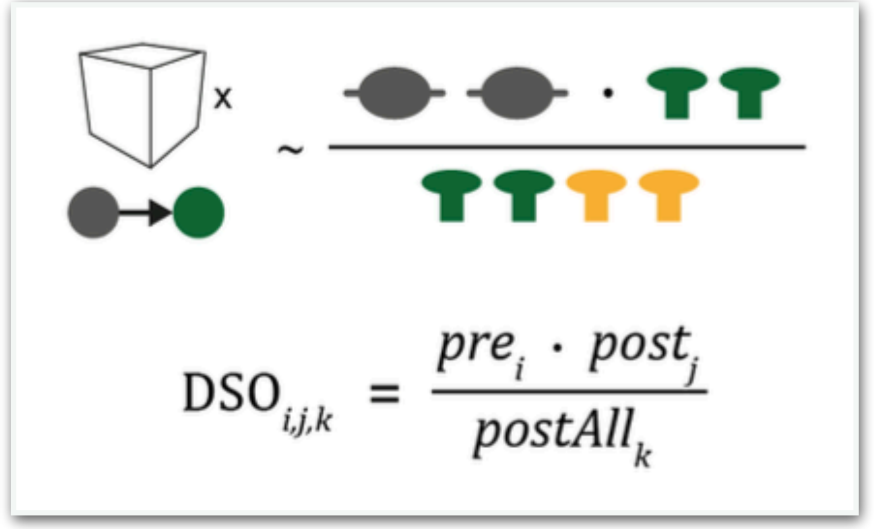
Outlook:

- Trainings: applied AI's SBI training
- Hackathons: 2024 Tübingen, 2025 Munich?
- Tutorial paper: Practitioners' guide to SBI
- Industry applications









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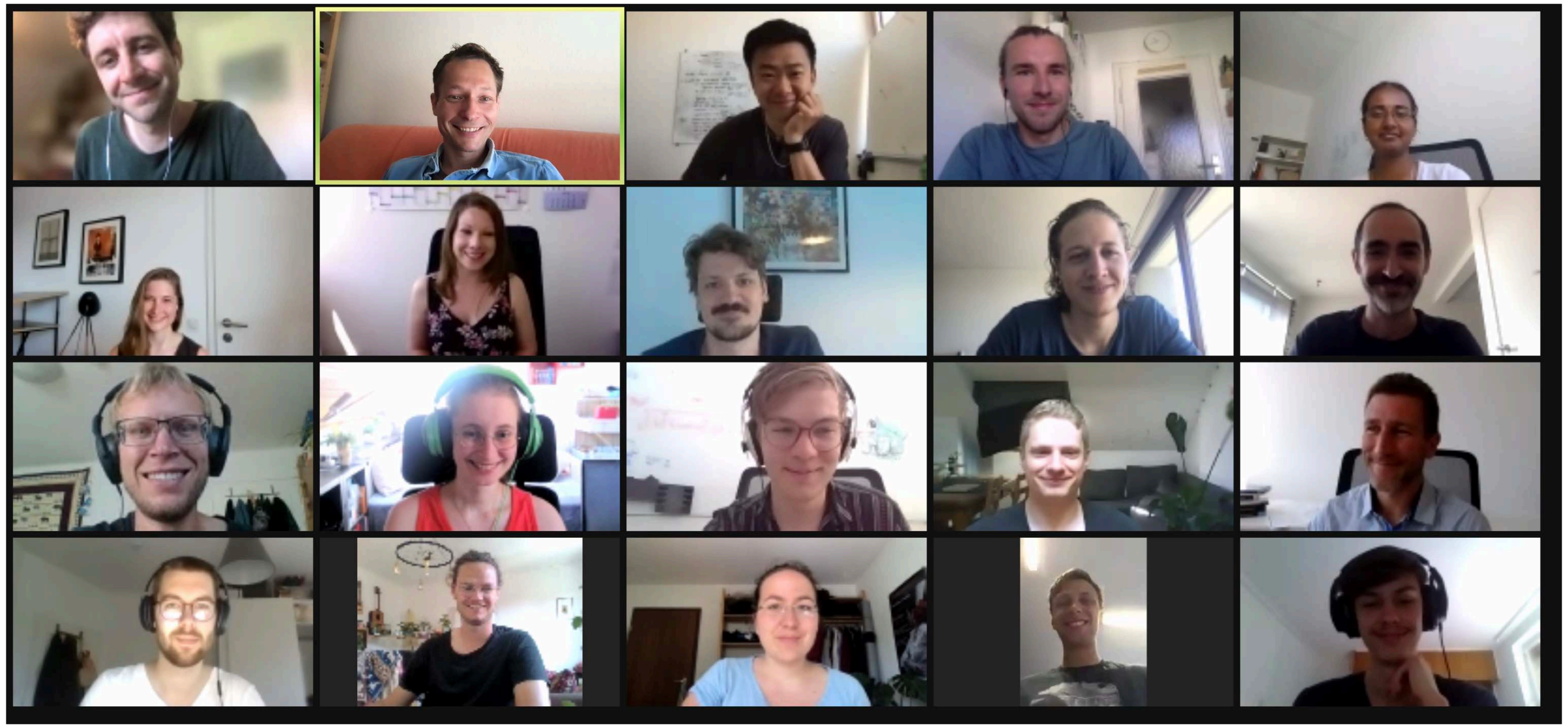

EBERHARD KARLS
UNIVERSITÄT
TÜBINGEN

Tübingen AI Center

MLS

SPP 2041
Computational
Connectomics

Bundesministerium
für Bildung
und Forschung

appliedAI institute for europe

Thank you!

Questions?

More info?
https://transferlab.ai/series/simulation-based-inference/