All-in-one simulation-based inference

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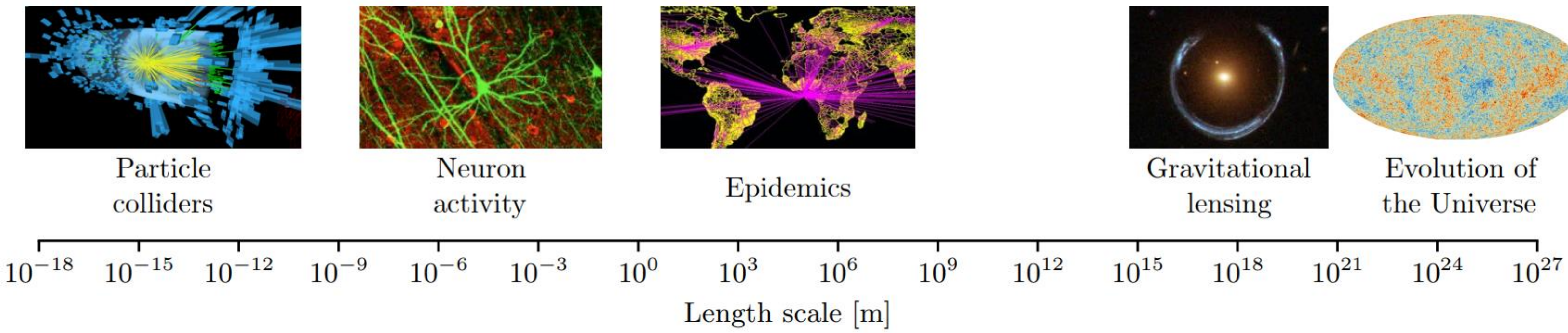
Challenge: Inference on scientific simulators



Credit: The frontier of simulation-based inference; Kyle Cranmer, Johann Brehmer and Gilles Louppe 2020

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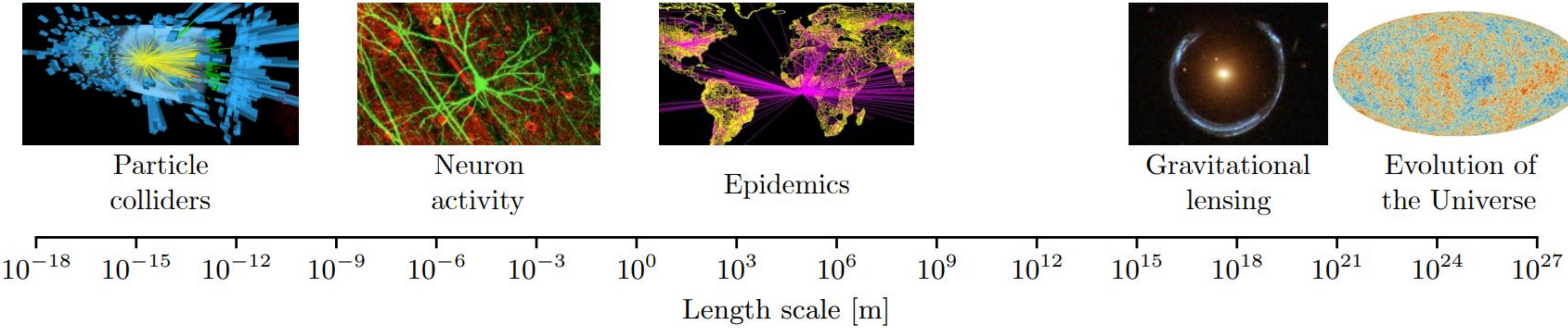

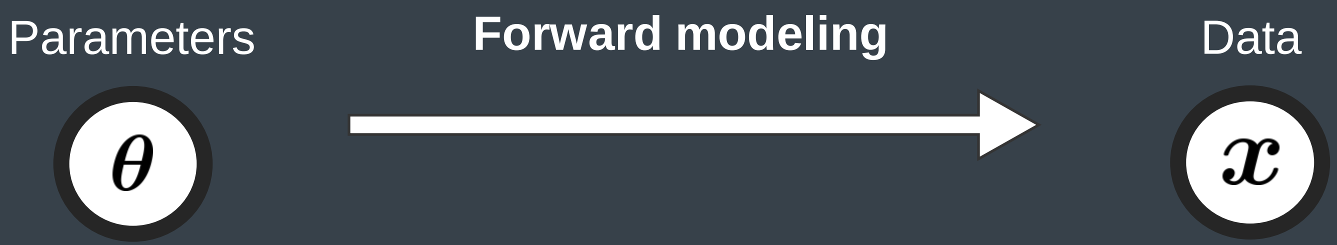

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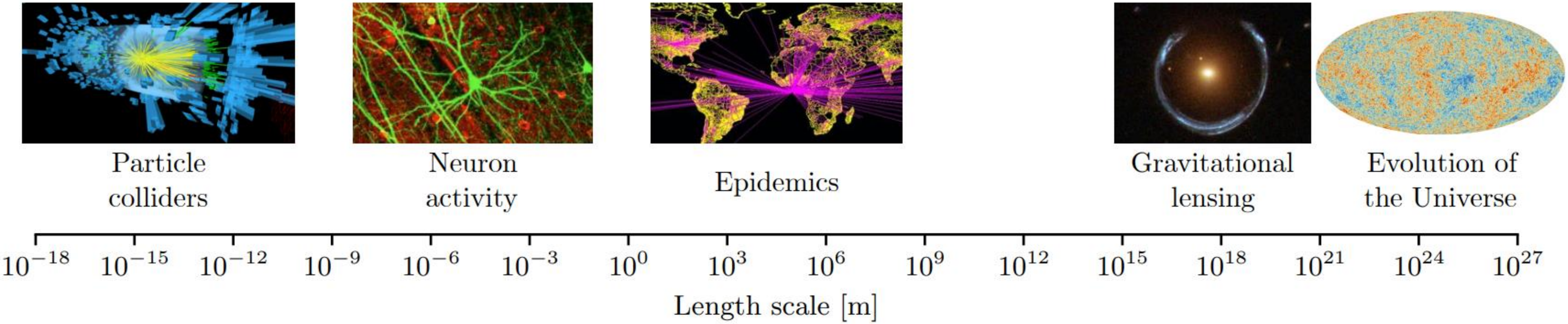

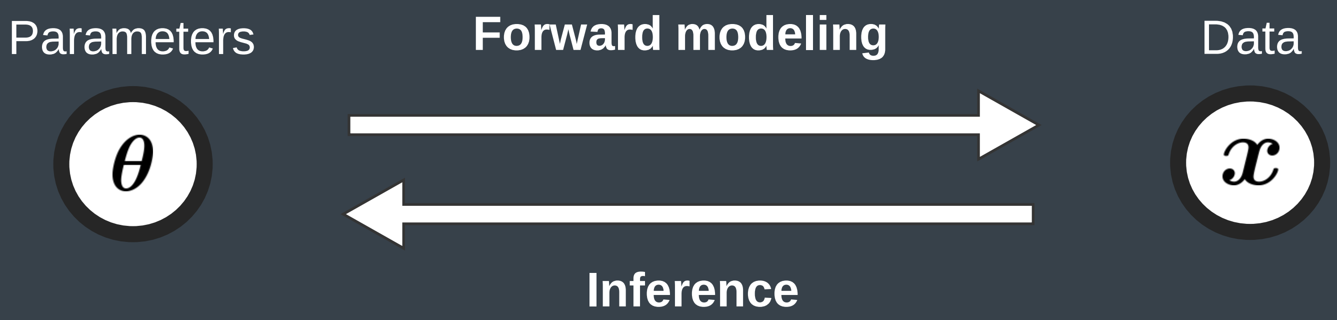

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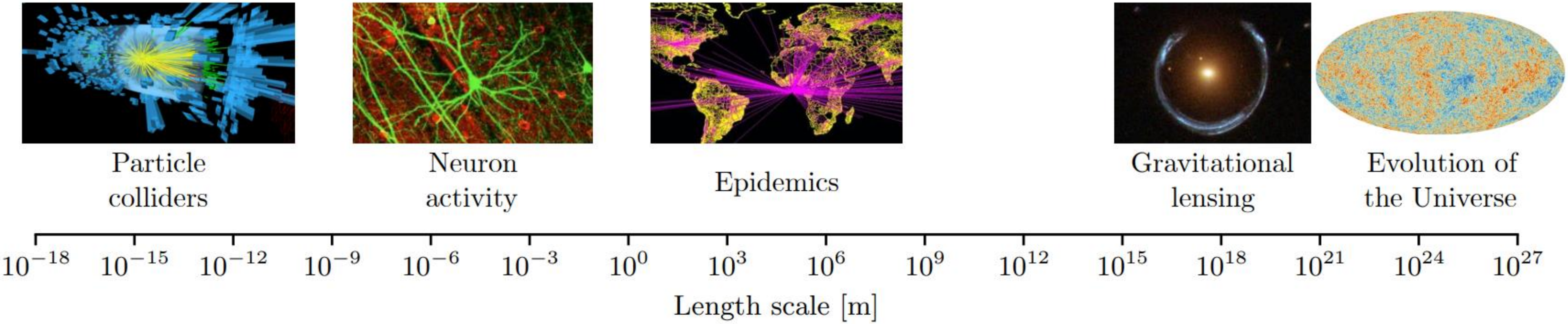

Parameters

Forward modeling

Data

Inference

- slow
- intractable likelihood
- non-differentiable

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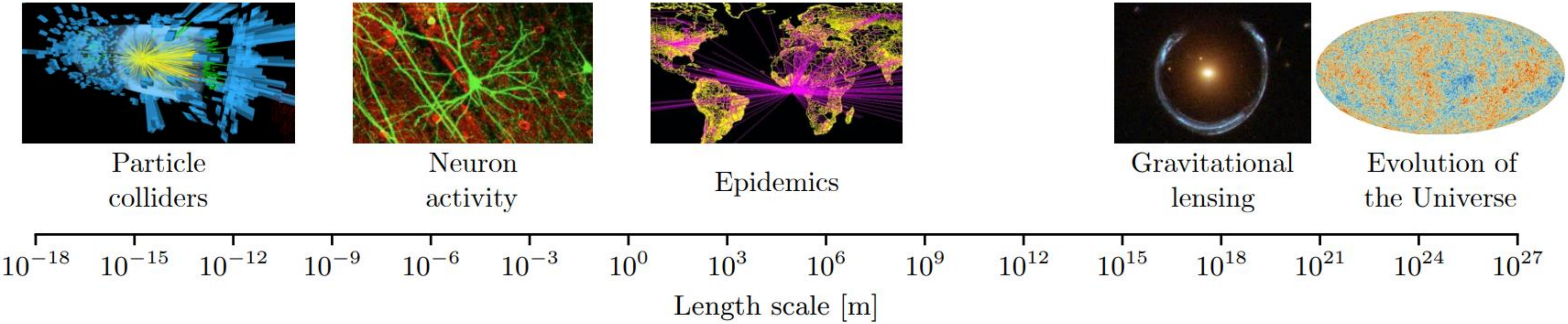


- slow
- intractable likelihood
- non-differentiable

Parameters

Forward modeling

Data

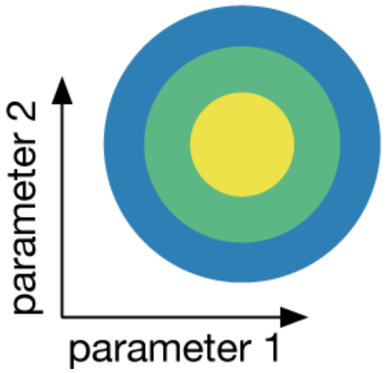
- MCMC not feasible
- MCMC is not **amortized**

Inference

Credit: The frontier of simulation-based inference; Kyle Cranmer, Johann Brehmer and Gilles Louppe 2020

Solution: Amortized simulation-based inference (SBI)

prior

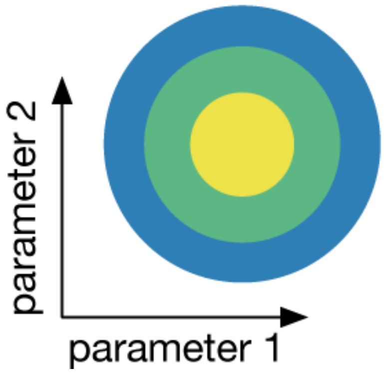


$$\boldsymbol{\theta} \sim p(\boldsymbol{\theta})$$

NPE (Neural posterior estimation)

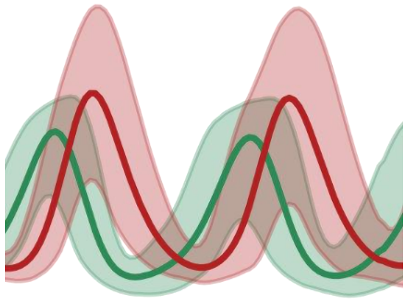
Solution: Amortized simulation-based inference (SBI)

prior



$$\boldsymbol{\theta} \sim p(\boldsymbol{\theta})$$

simulated data

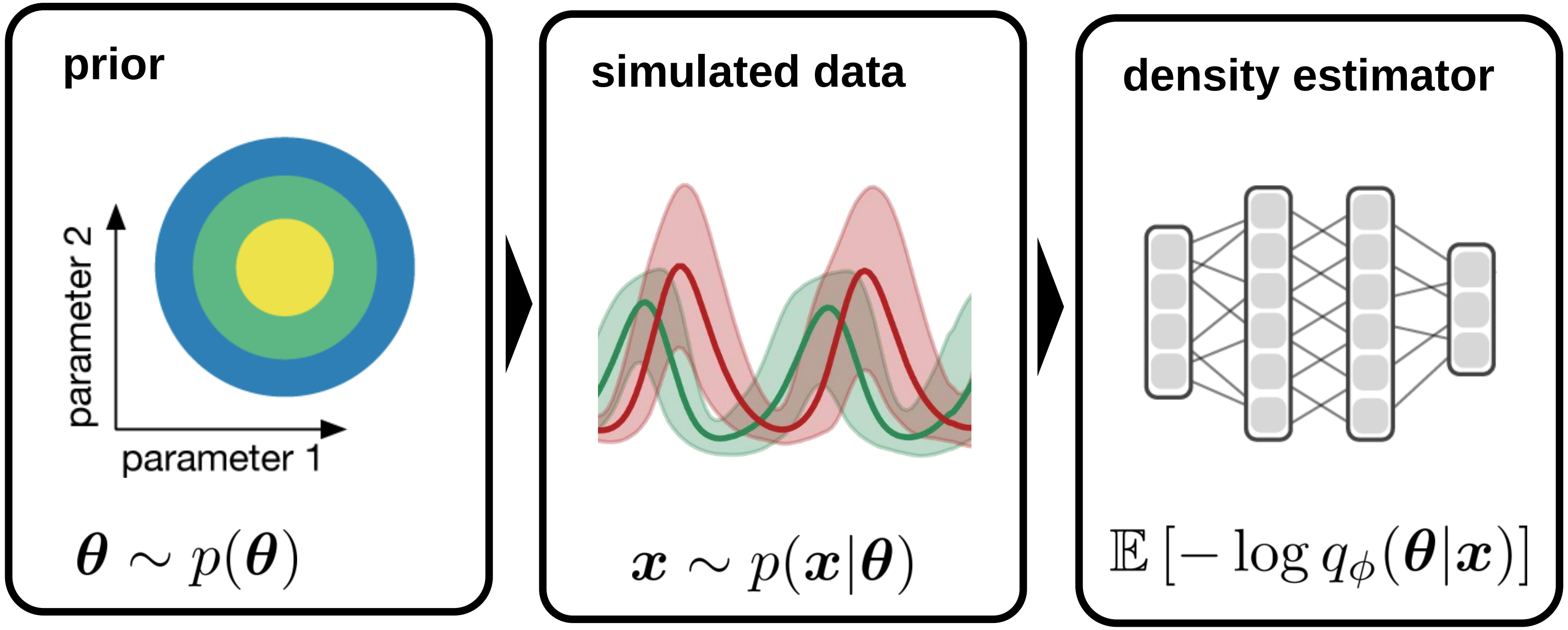


$$\boldsymbol{x} \sim p(\boldsymbol{x}|\boldsymbol{\theta})$$

NPE (Neural posterior estimation)

Papamakarios, G., & Murray, I. (2016); Lueckmann et al. (2017);

Solution: Amortized simulation-based inference (SBI)



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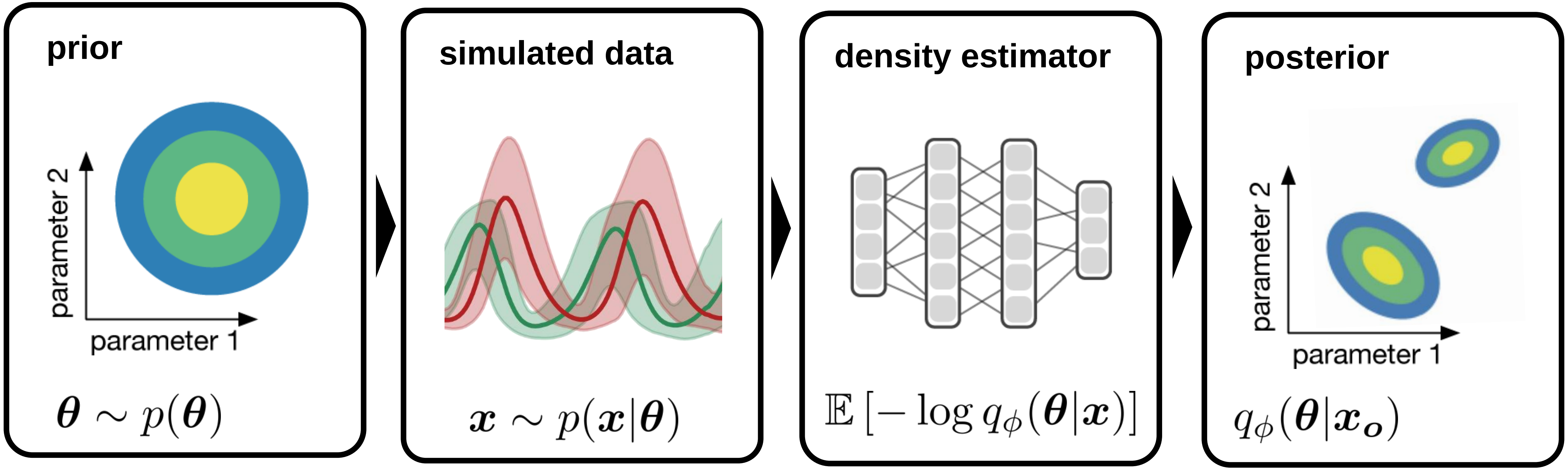
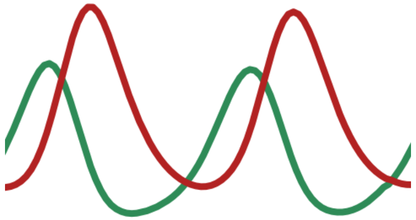


NPE (Neural posterior estimation)

$\boldsymbol{x_o}$



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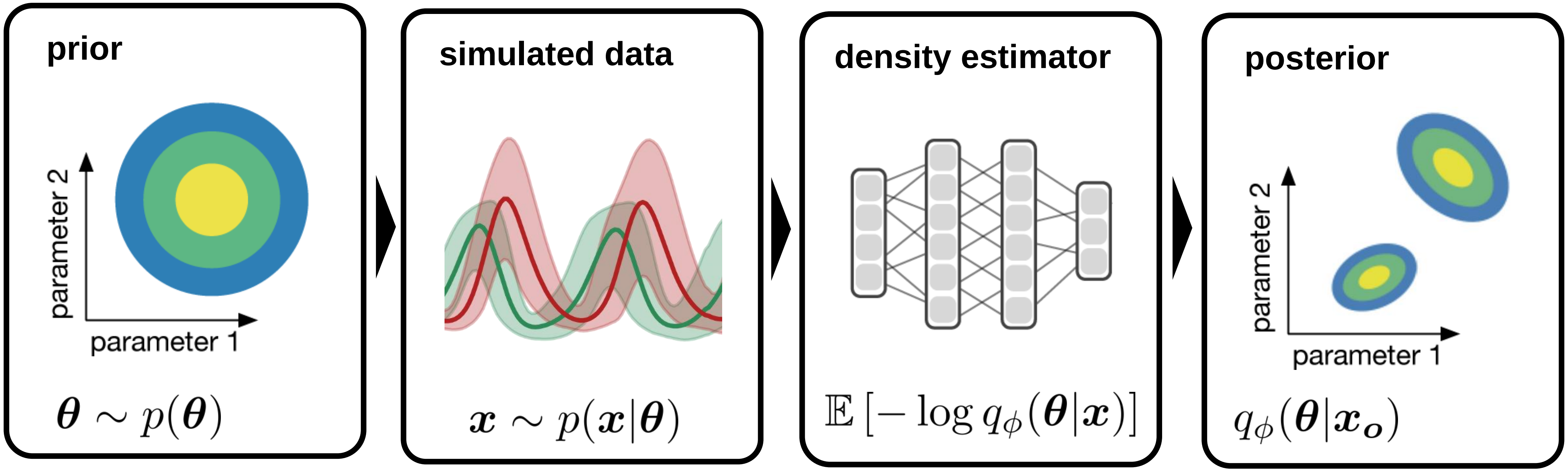

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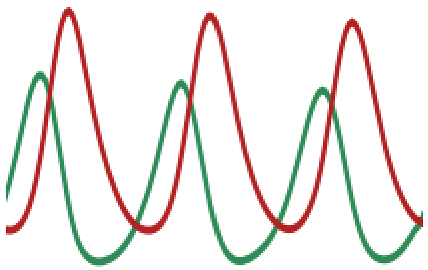

Papamakarios, G., & Murray, I. (2016); Lueckmann et al. (2017);

Limitations of current simulation-based inference methods

Parameters

Data

Simulator

Inference

Limitations of current simulation-based inference methods

Parameters

Data

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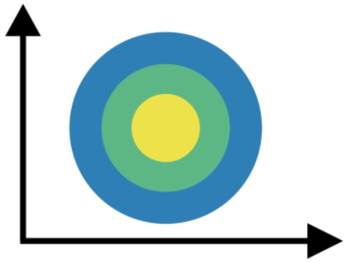
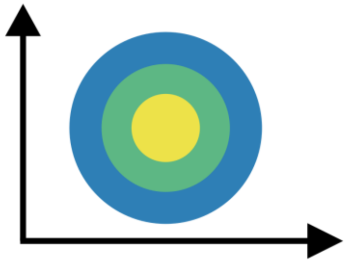
Inference

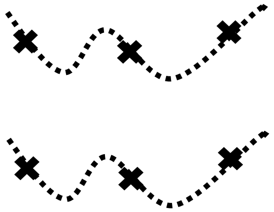
Requires fixed prior and finite number of parameters



Limitations of current simulation-based inference methods

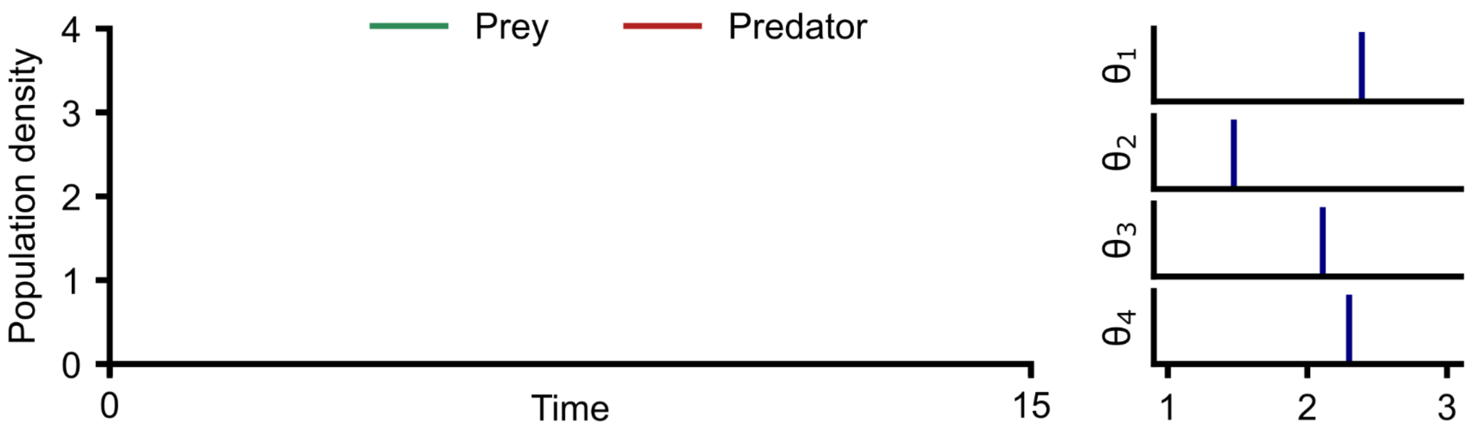
Parameters	Data	Simulator	Inference
Requires fixed prior and finite number of parameters	Must be structured and complete e.g., static sized vectors		





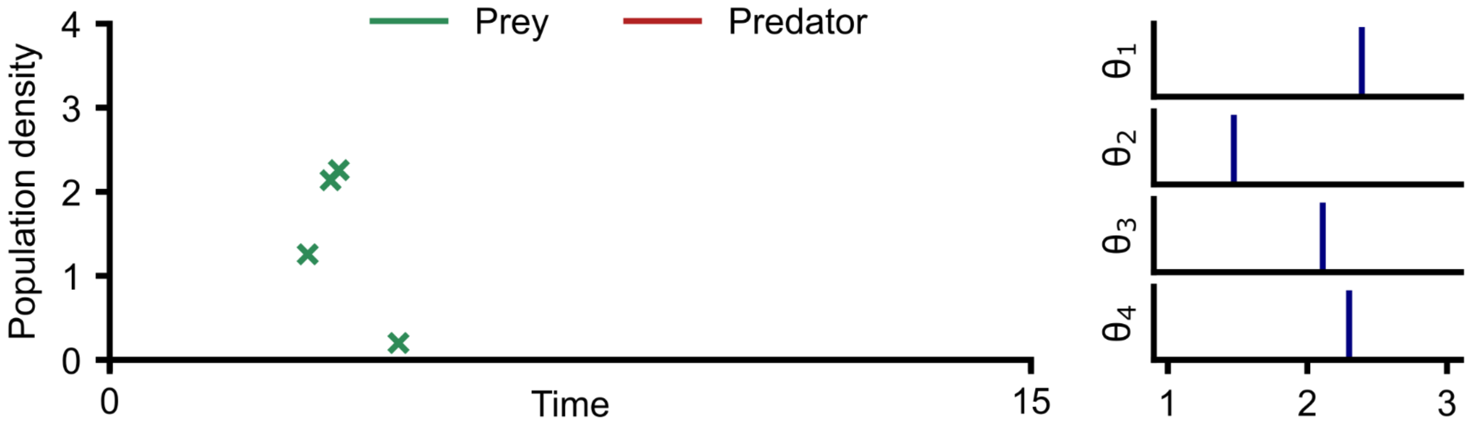
Example: Lotka Volterra

- Predator-Prey dynamics



Example: Lotka Volterra

- Predator-Prey dynamics
- Observations can happen at *any point in time*
- Missing data



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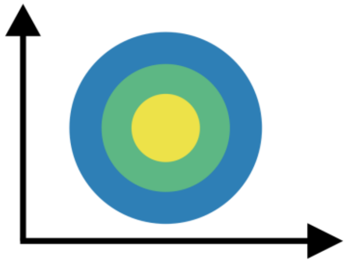

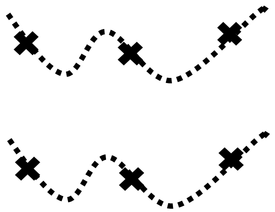

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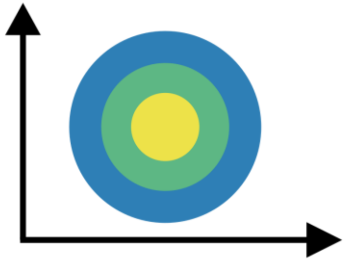
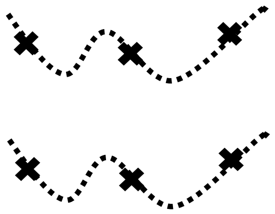


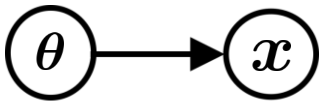
Data

Must be structured and complete



Simulator

Requires many simulations to train



A **black-box** that can generate data from parameters

Inference

Limitations of current simulation-based inference methods

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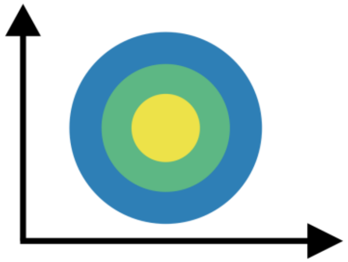

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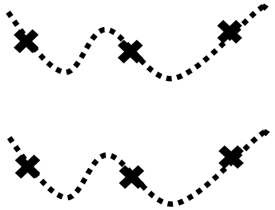

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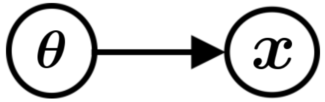
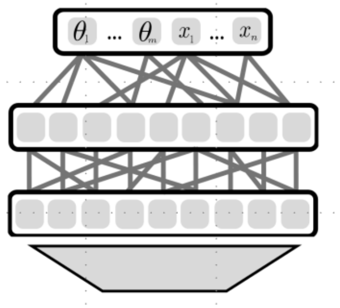


A **black-box** that can generate data from parameters

Inference

User must select specific inference task



posterior $p(\boldsymbol{\theta} \mid \boldsymbol{x})$ **NPE**

likelihood $p(\boldsymbol{x} \mid \boldsymbol{\theta})$ **NLE**

Limitations of current simulation-based inference methods

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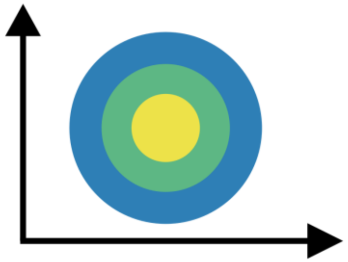

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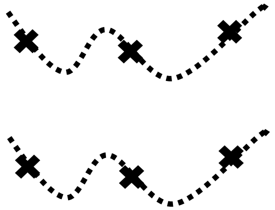

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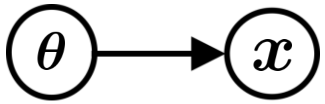

A **black-box** that can generate data from parameters

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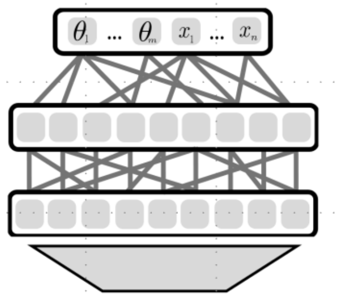


posterior $p(\boldsymbol{\theta} \mid \boldsymbol{x})$ **NPE**

likelihood $p(\boldsymbol{x} \mid \boldsymbol{\theta})$ **NLE**

These **inflexibilities** prevents application of SBI an many real-world problems

We developed the Simformer a single method to tackle **all of these limitations at once.**

Simformer: All-in-one simulation-based inference

Parameters

Data

Simulator

All-in-1-inference

Simformer: All-in-one simulation-based inference

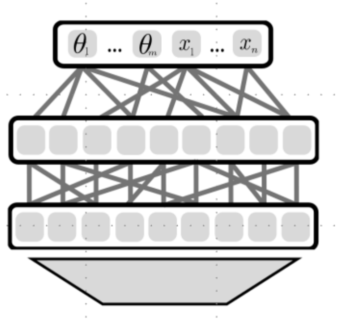
Parameters

Data

Simulator

All-in-1-inference

Learn all inference or emulation tasks



posterior $p(\boldsymbol{\theta} \mid \boldsymbol{x})$

likelihood $p(\boldsymbol{x} \mid \boldsymbol{\theta})$

any conditional

$$p(\theta, x_2 \mid x_1)$$

Simformer: All-in-one simulation-based inference

Parameters

Data

Handles missing or unstructured data

Simulator

All-in-1-inference

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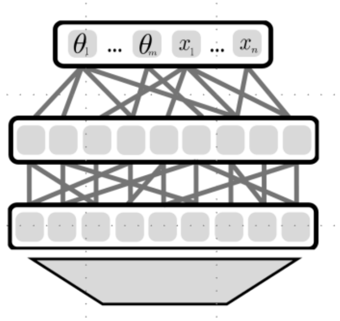

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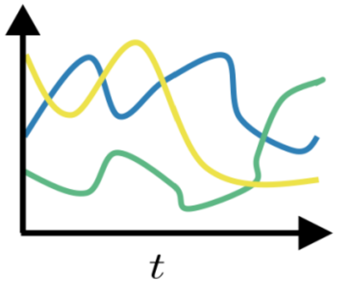
Simformer: All-in-one simulation-based inference

Parameters

Functional parameters



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Simulator

All-in-1-inference

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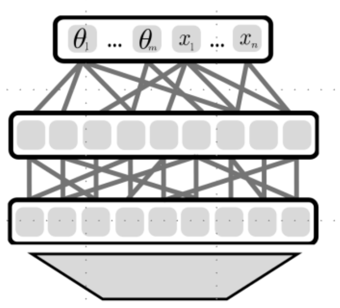

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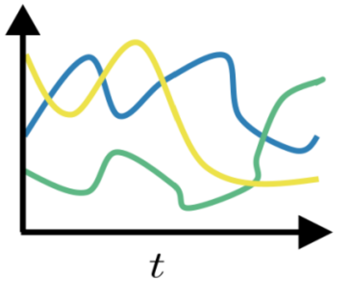
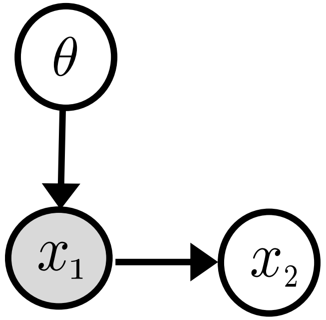


Data

Handles missing or unstructured data

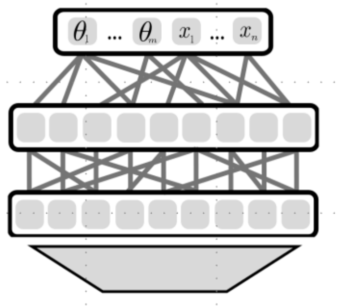
Simulator

Can exploit structure to increase simulation efficiency



All-in-1-inference

Learn all inference or emulation tasks



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Simformer: All-in-one simulation-based inference

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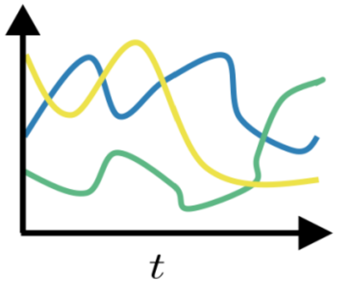
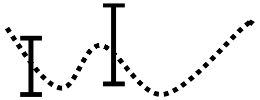


Post-hoc modifications

Data

Handles missing or unstructured data

Abstract constraints e.g. observation intervals



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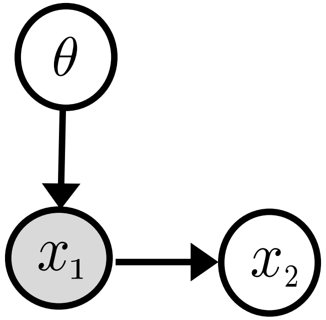
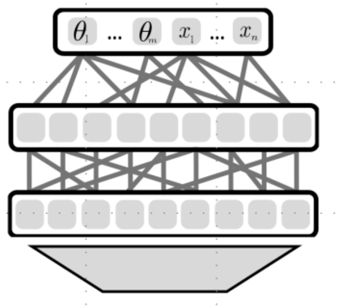


All-in-1-inference

Learn all inference or emulation tasks



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Simformer: Transformer + Diffusion model

transformer **diffusion model**

$$p(\theta, x_2 | x_1)$$

$$\underset{\hat{\mathbf{x}}}{\begin{pmatrix} \theta \\ x_1 \\ x_2 \end{pmatrix}} \qquad \underset{M_C}{\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}}$$

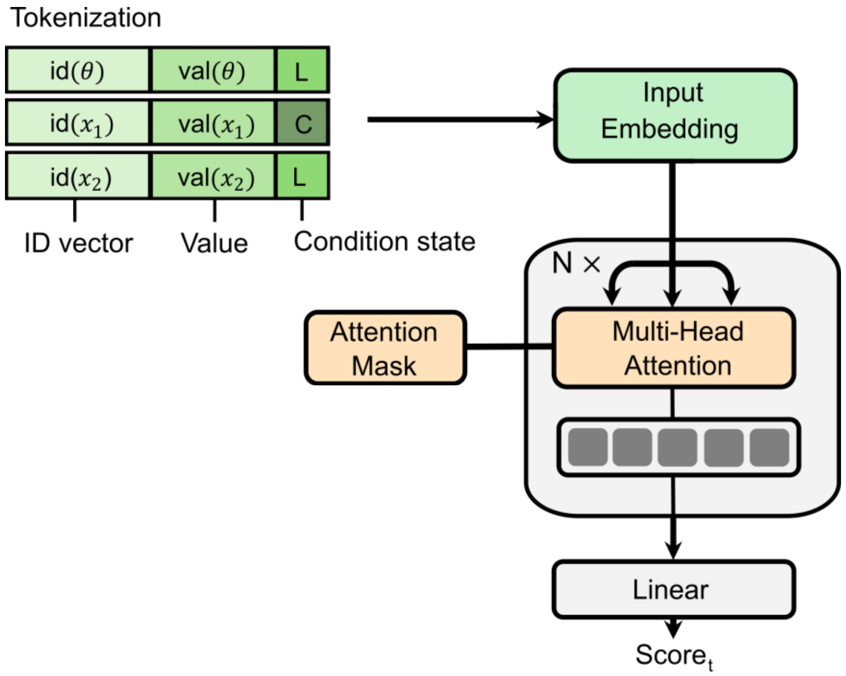
Simformer: Transformer + Diffusion model

transformer

diffusion model

$$p(\theta, x_2 | x_1)$$

$$\hat{\mathbf{x}} = \begin{pmatrix} \theta \\ x_1 \\ x_2 \end{pmatrix} \quad M_C = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$$



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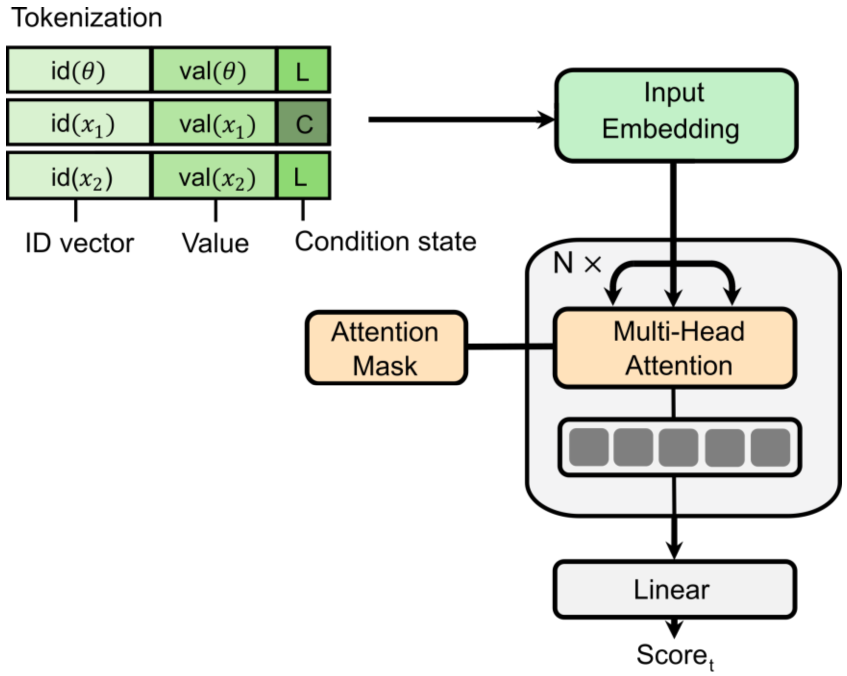

Handles missing or unstructured data

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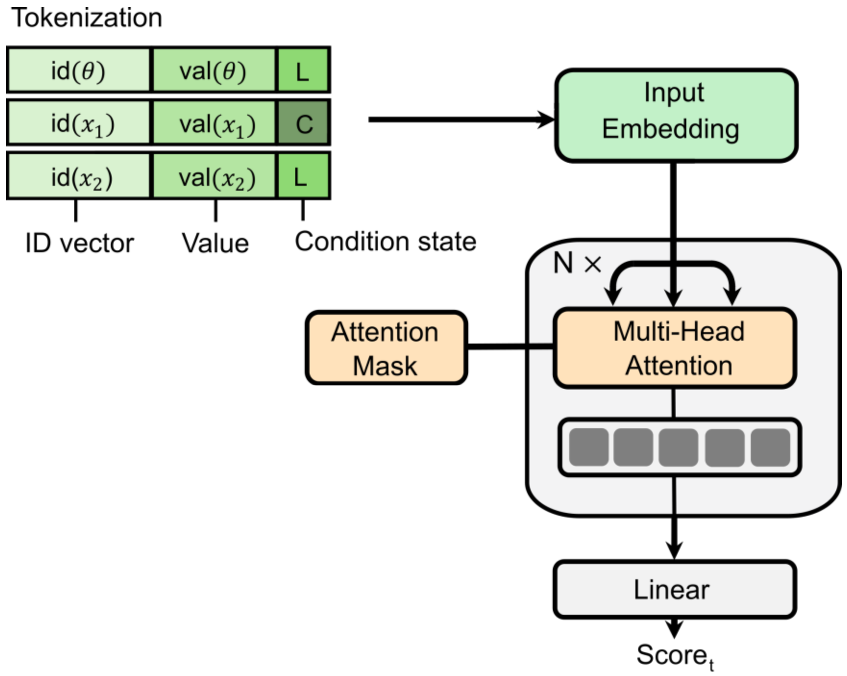

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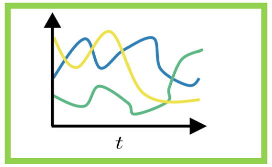

Functional parameters

Simformer: Transformer + Diffusion model

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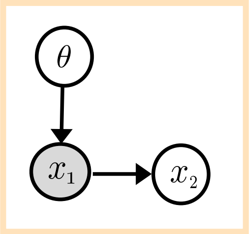
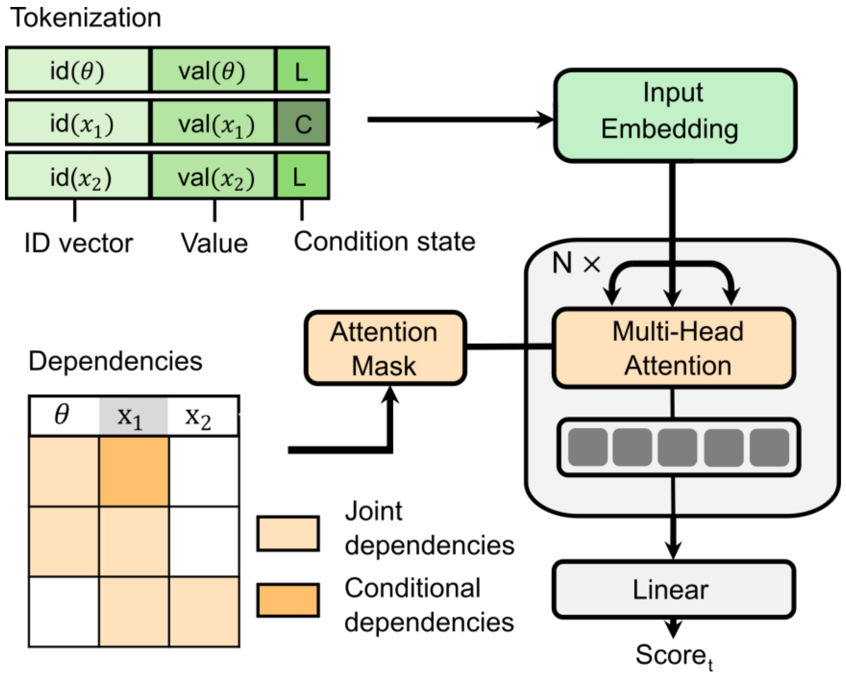


dependencies



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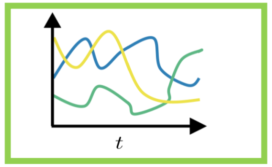

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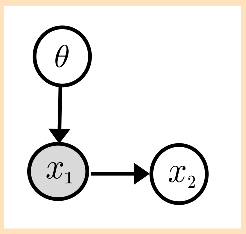
$\hat{\mathbf{x}}$ $\quad$ M_C



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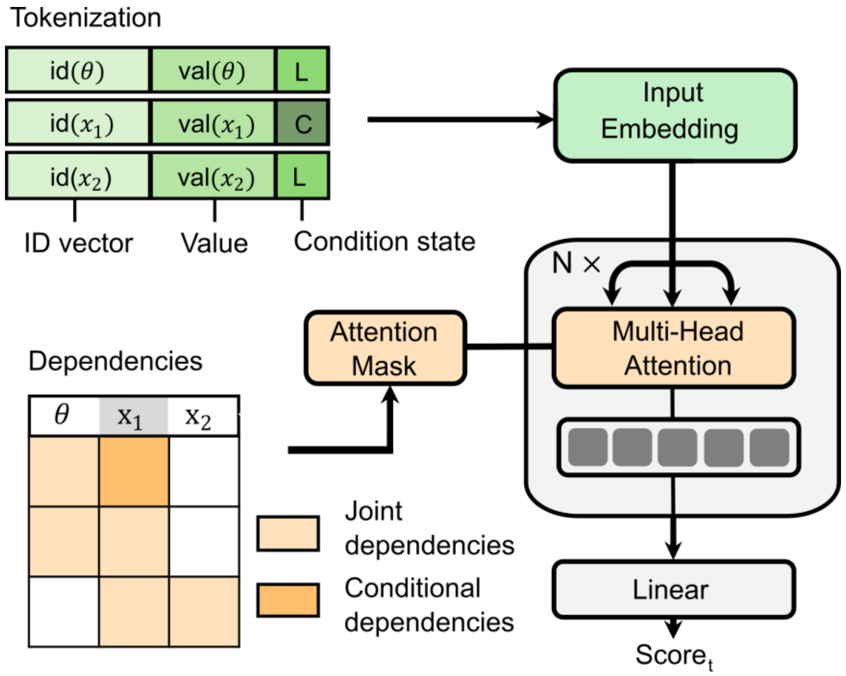

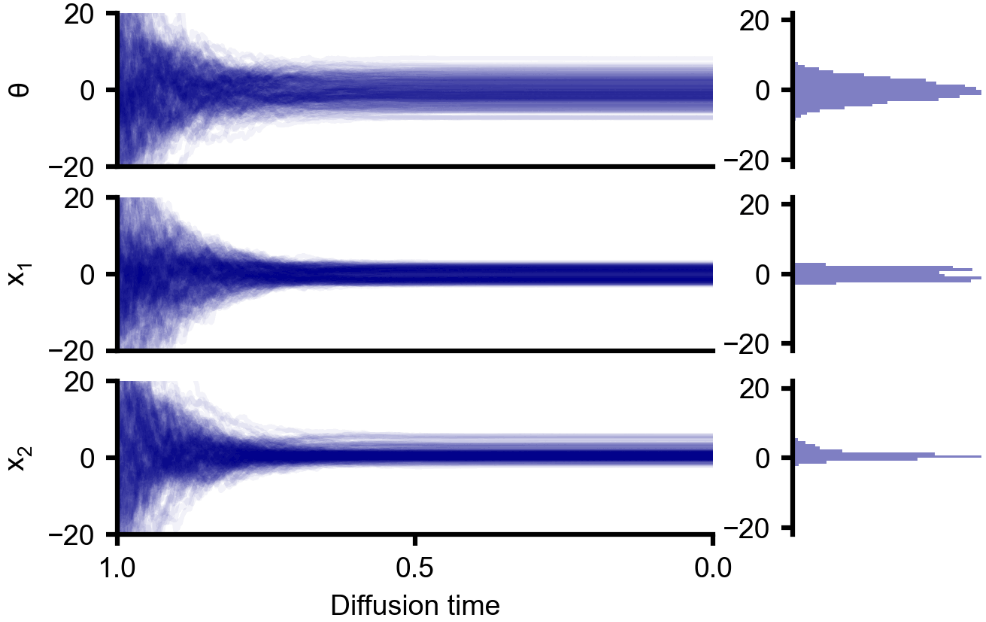

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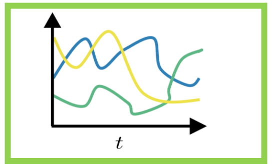
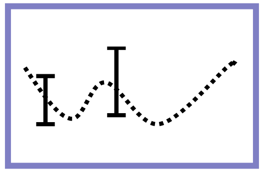
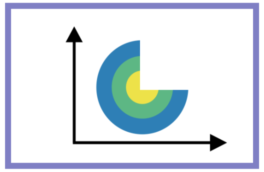


Functional parameters



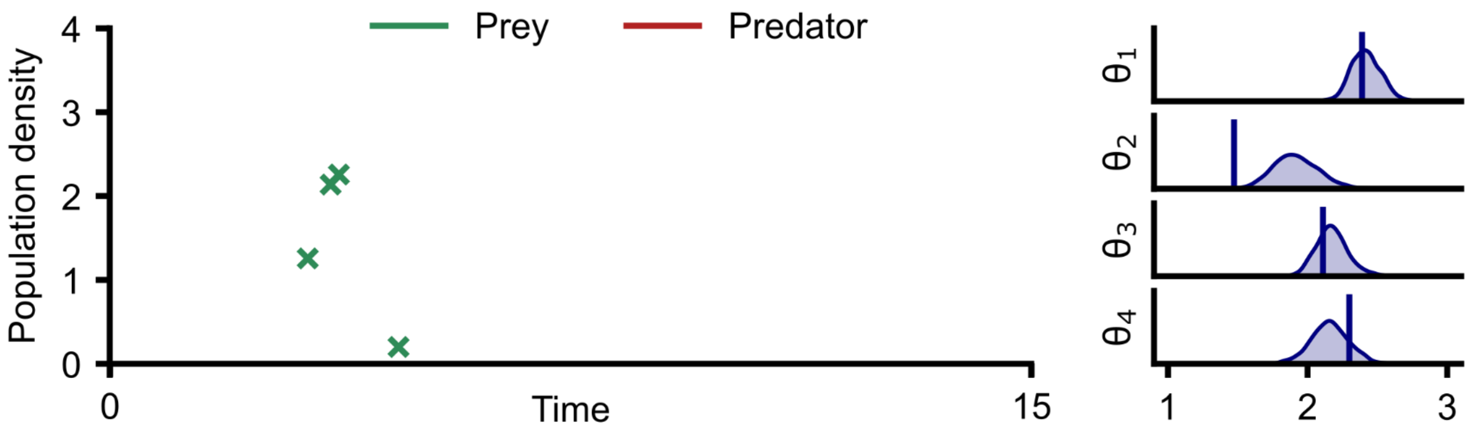
obs. intervals



post-hoc mod.

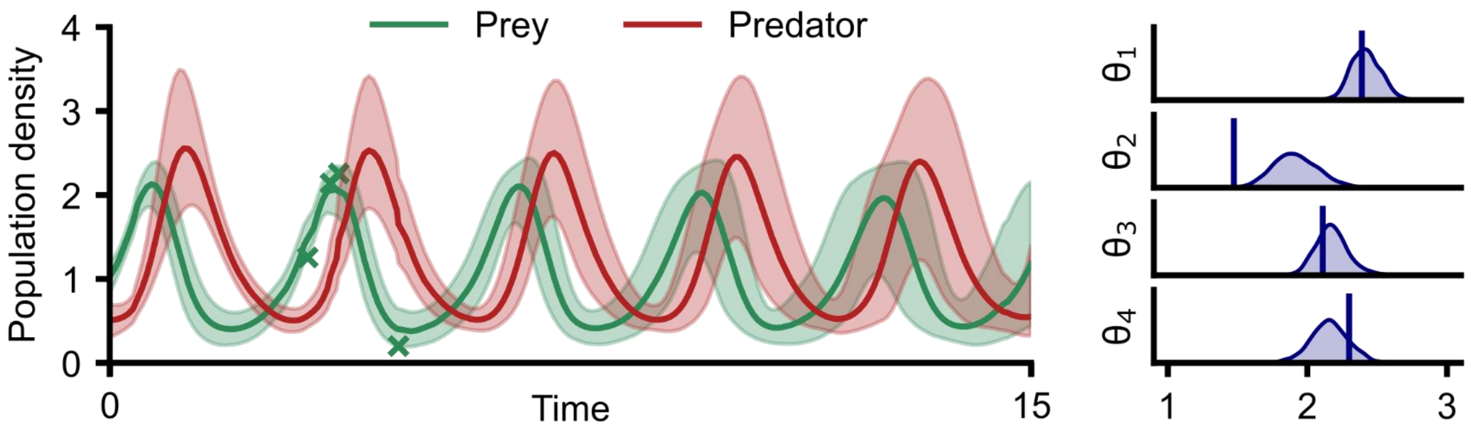
Example: Lotka Volterra

- Predator-Prey dynamics
- Observations can happen at *any point in time*
- Missing data



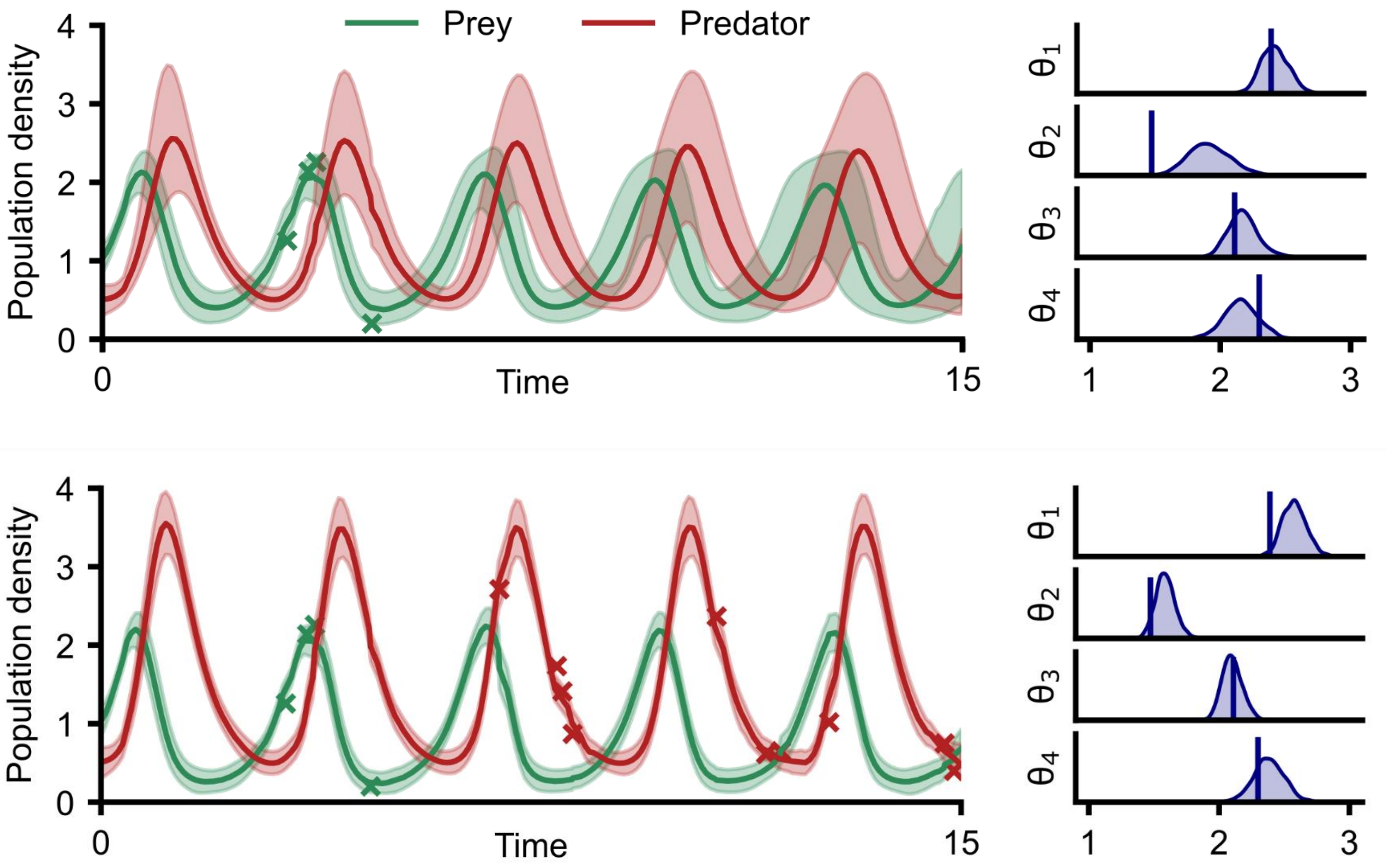
Example: Lotka Volterra

- Predator-Prey dynamics
- Observations can happen at *any point in time*
- Missing data
- Simultaneous inference and predictive estimation



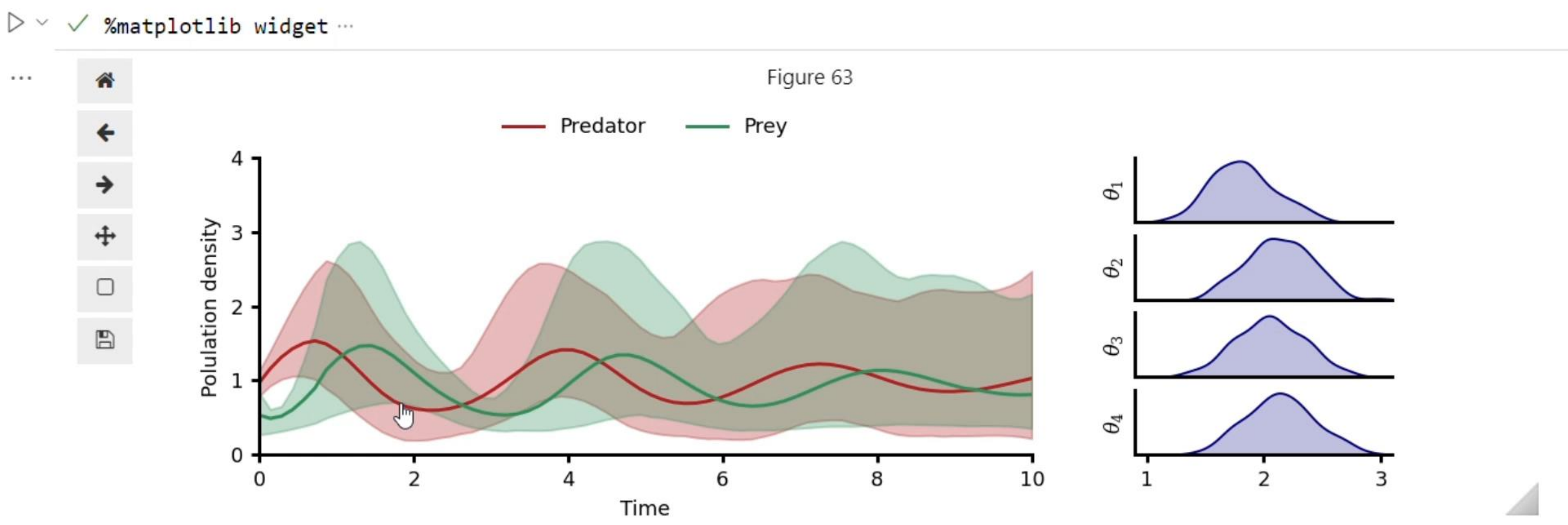
Example: Lotka Volterra

- Predator-Prey dynamics
- Observations can happen at *any point in time*
- Missing data
- Simultaneous inference and predictive estimation
- Add *additional* observations



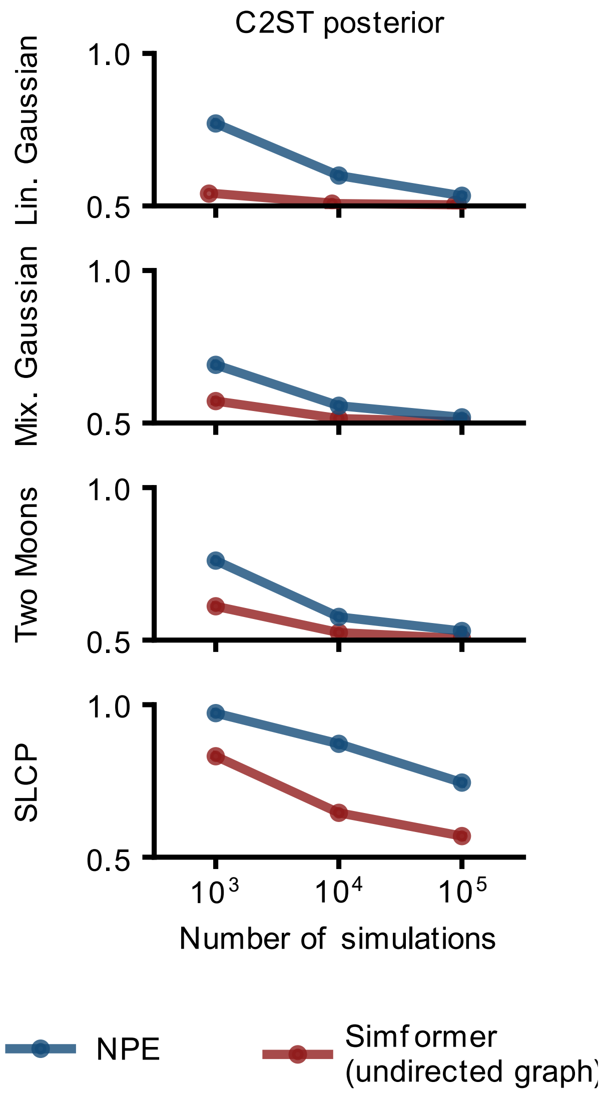
Simformer allows real-time interactive inference

Simformer allows real-time interactive inference



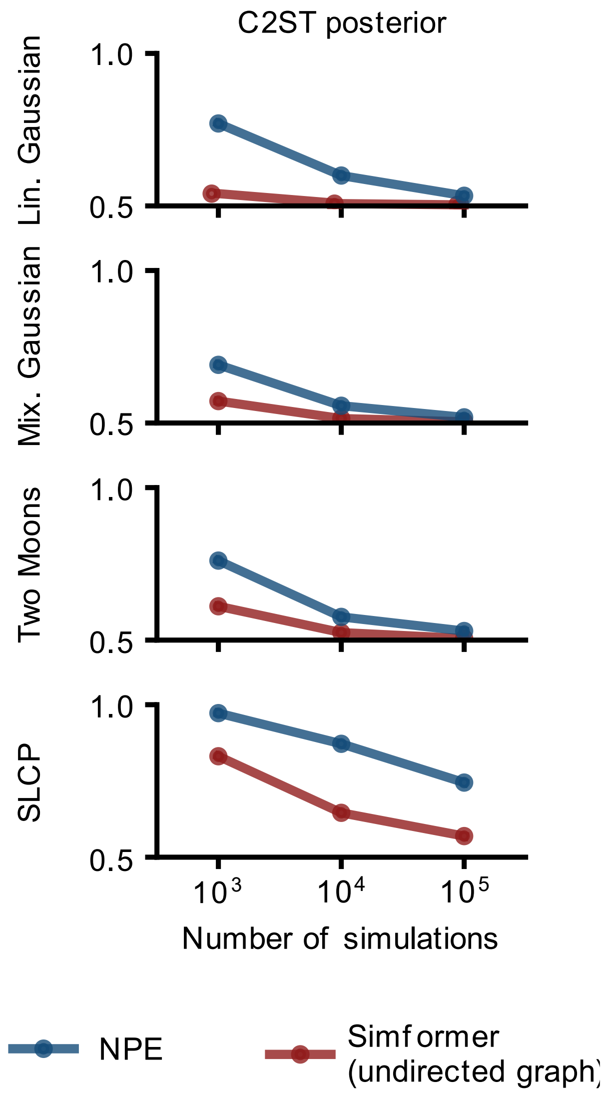
Simformer is flexible and accurate

- At least as accurate as specialized methods on posterior estimation, despite learning **all conditionals.**



Simformer is flexible and accurate

- At least as accurate as specialized methods on posterior estimation, despite learning **all conditionals.**
- Exploiting known structure can boost simulation efficiency in tasks with sparse dependencies.



All-in-one simulation-based inference

Manuel Gloeckler Michael Deistler Christian Weilbach Frank Wood Jakob H. Macke





Paper:

https://arxiv.org/abs/2404.09636

Code:

https://github.com/mackelab/simformer

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