Bayesian calibration of differentiable agent-based models

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AI4ABM workshop — ICLR 2023

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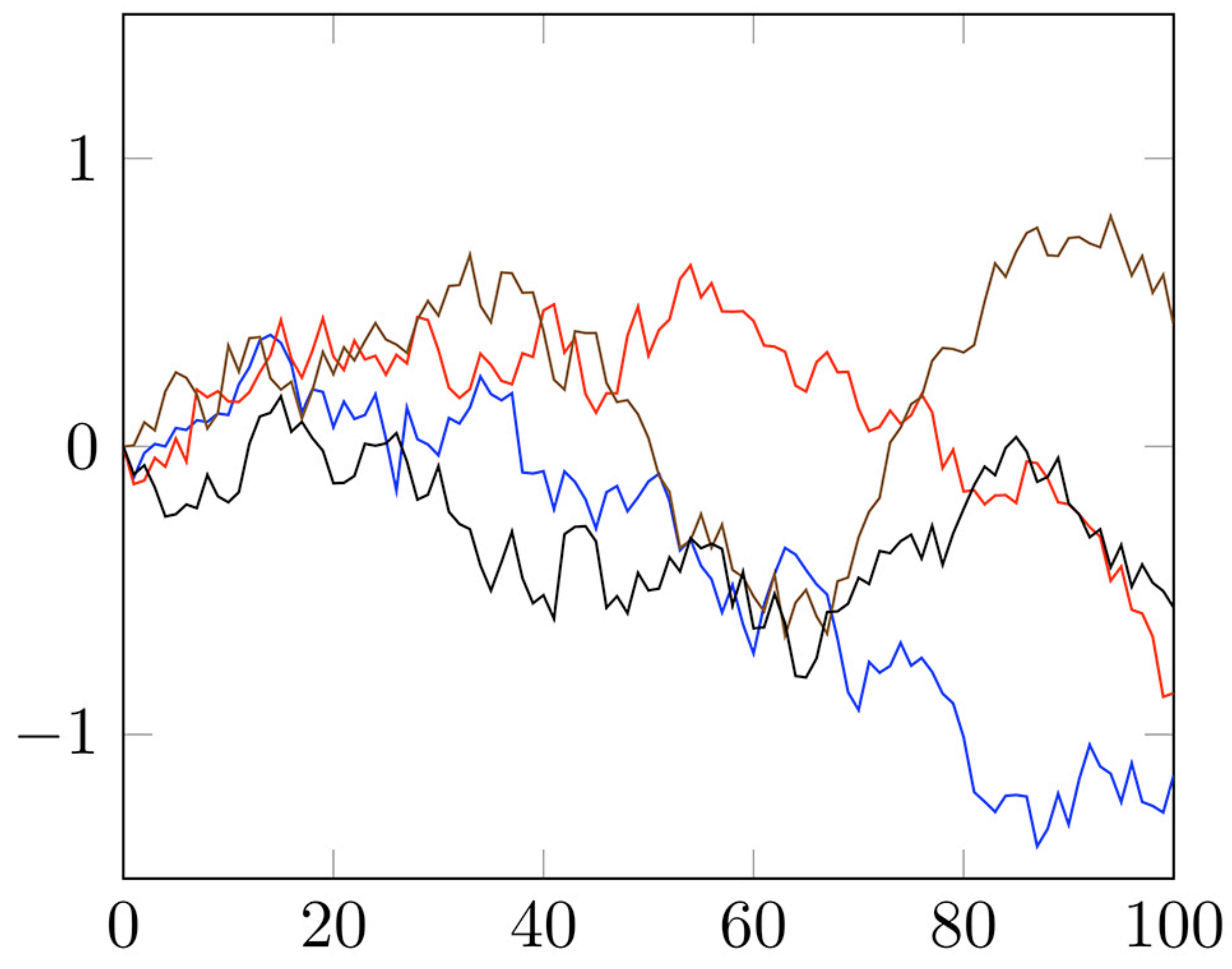
Calibration of ABMs

- Forward simulation:

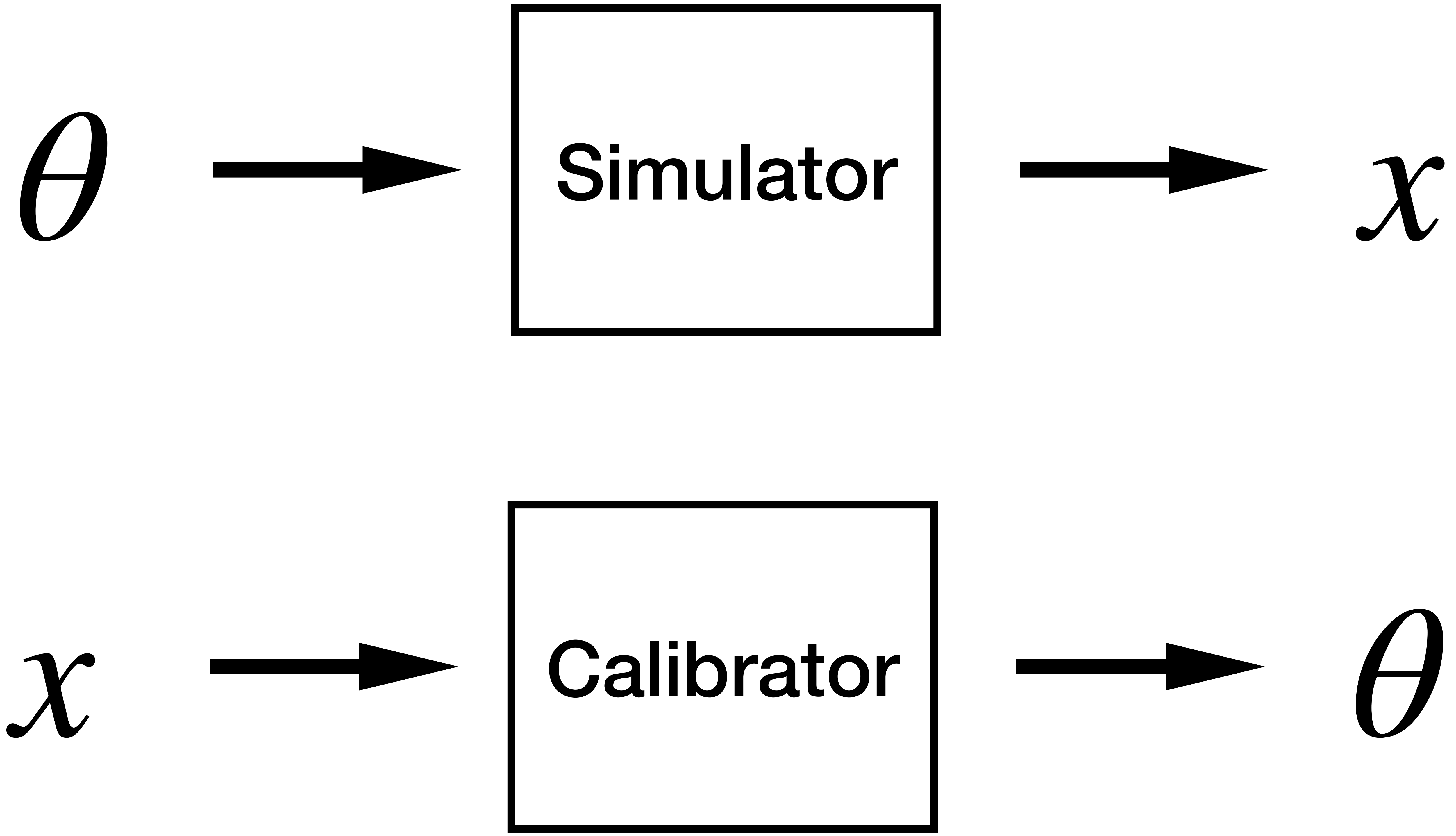
θ → **ABM simulator** → x

ABM parameters



ABM calibration aims to invert this process

Calibration of ABMs



Why is it hard?

- Expensive simulator

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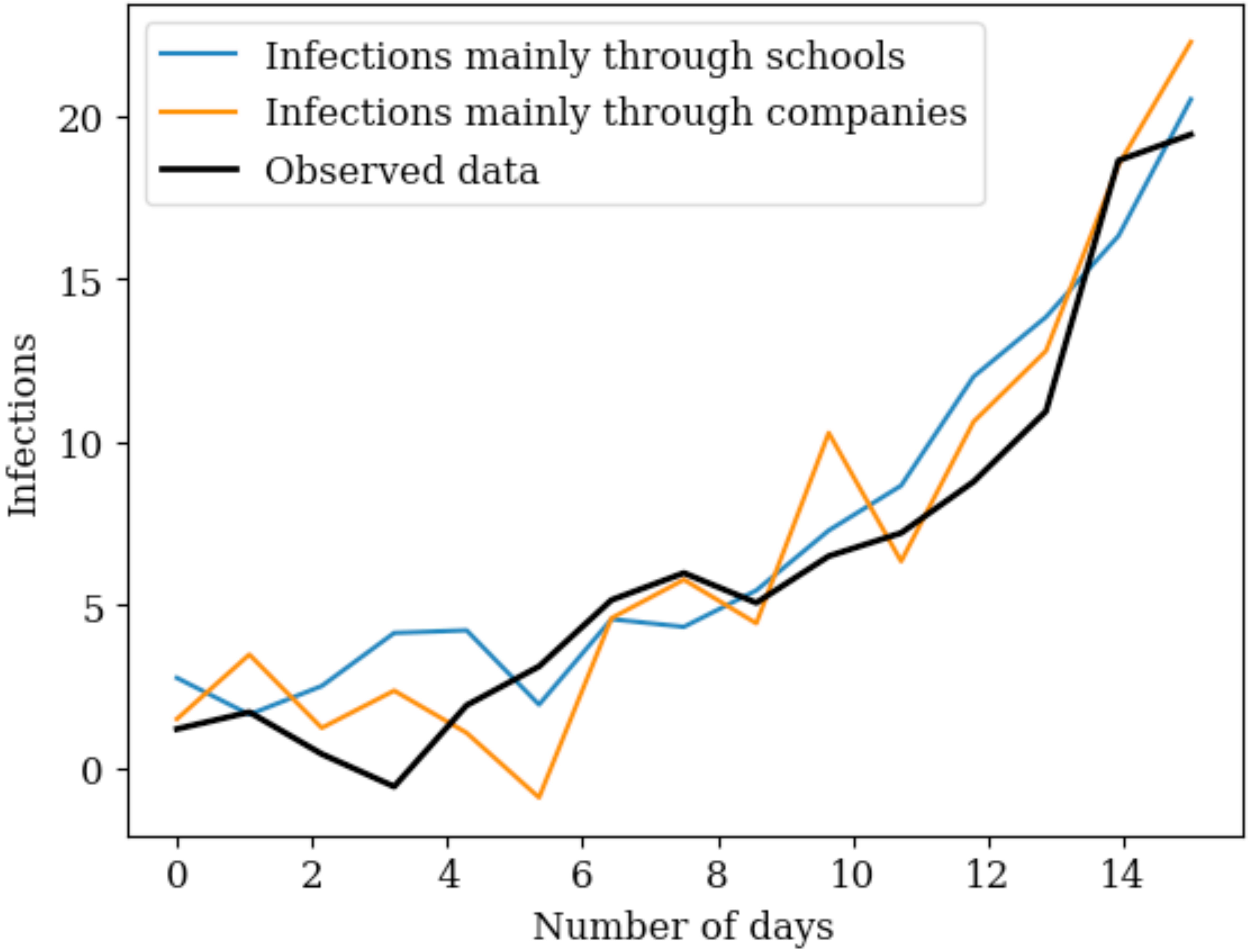
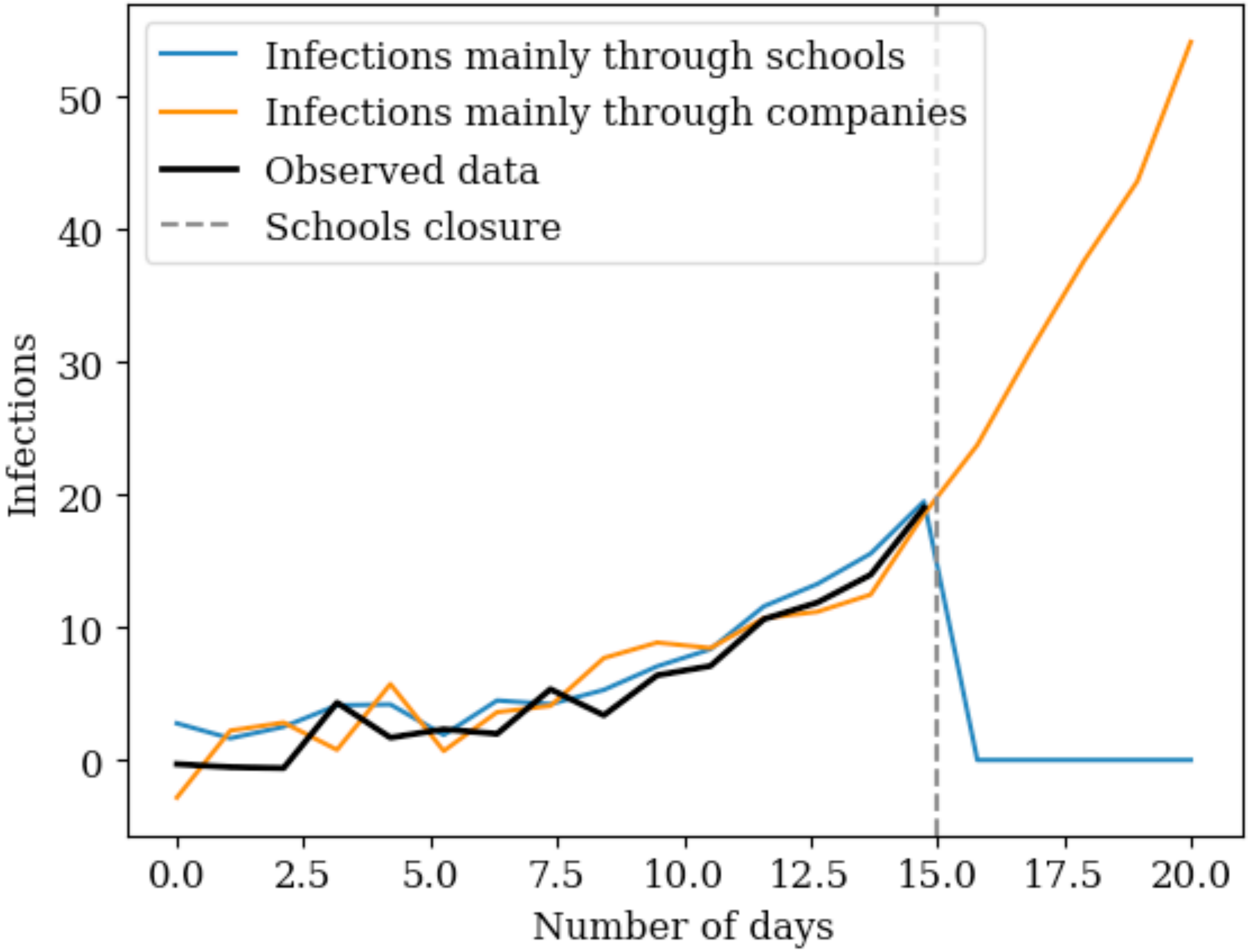
- Large parameter space

Calibration of ABMs

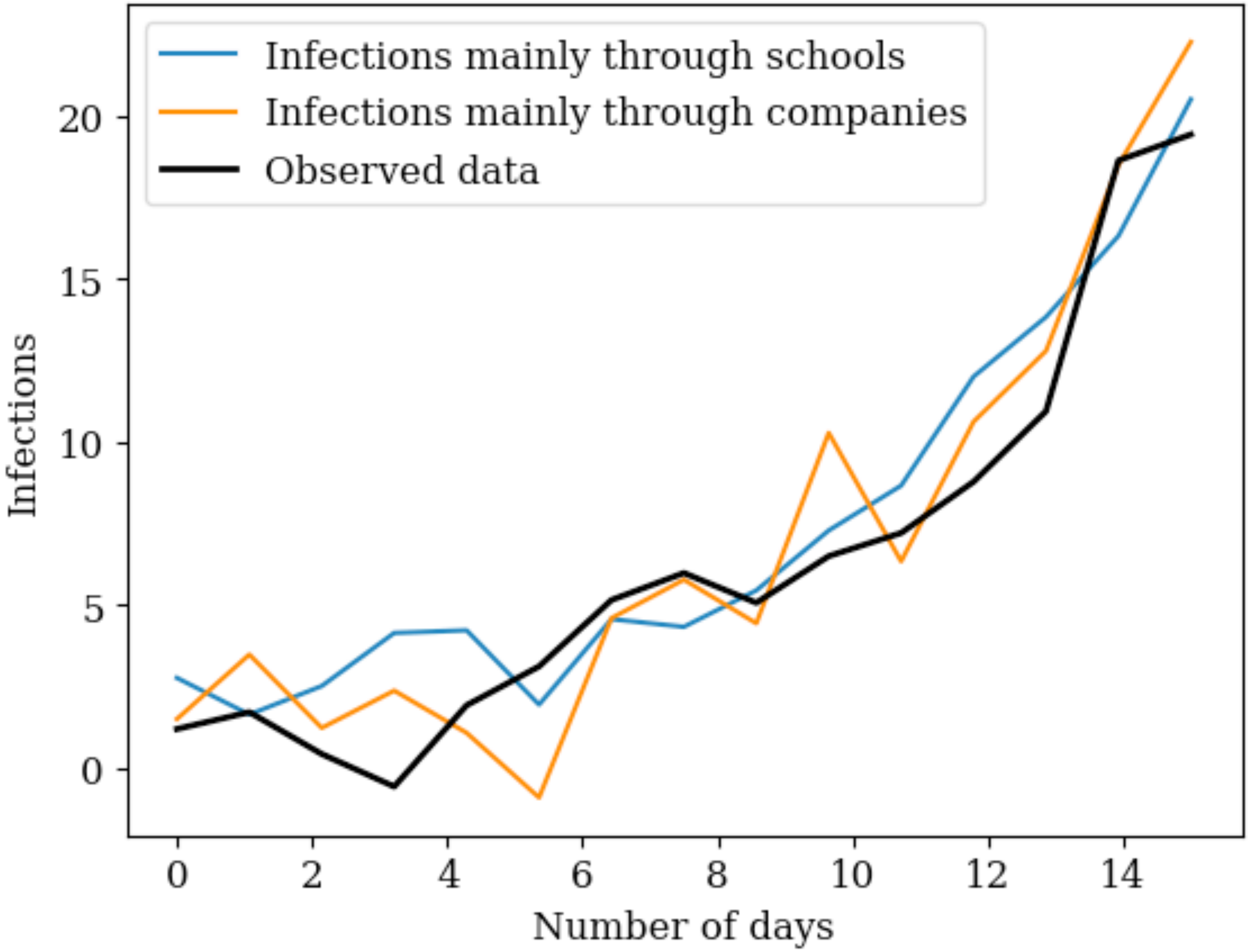
1. Uncertainty quantification





Calibration of ABMs

2. Expert (prior) knowledge

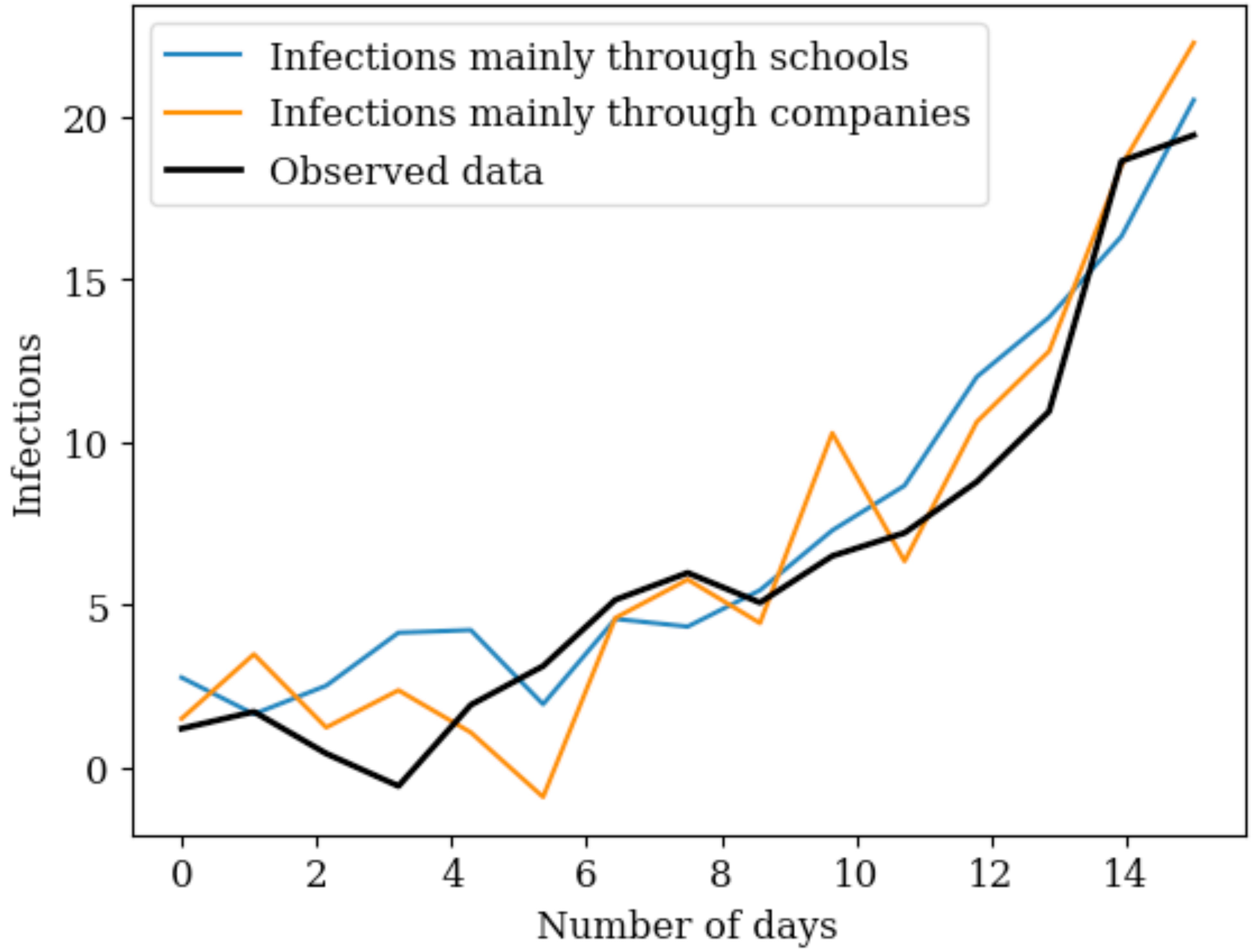


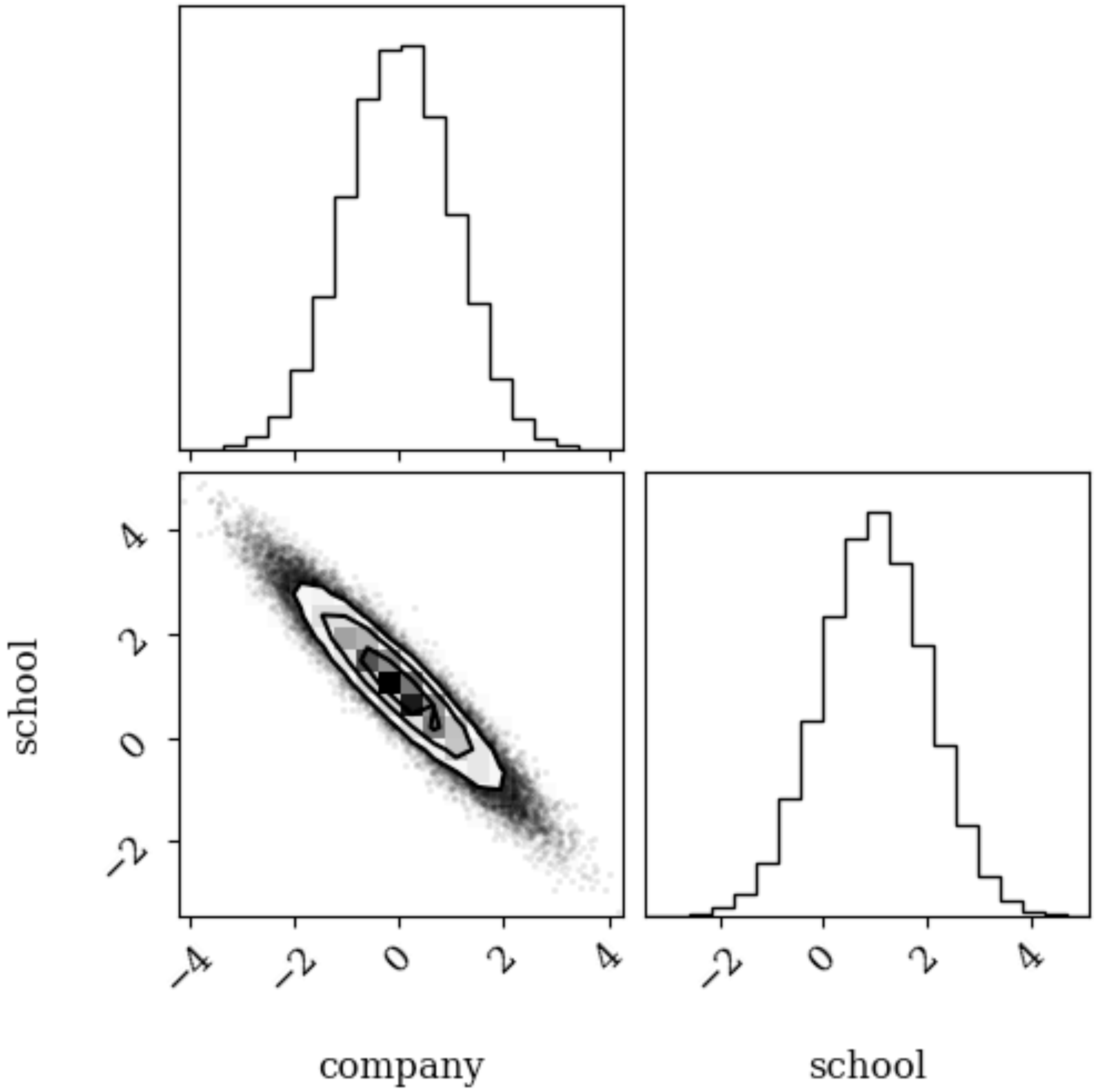
Need to include prior information in our calibration process

Bayesian calibration

Allows to tackle both problems

$$\underbrace{p(\theta|x)}_{\text{posterior}} \propto \underbrace{p(x|\theta)}_{\text{likelihood}}\ \underbrace{p(\theta)}_{\text{prior}}$$



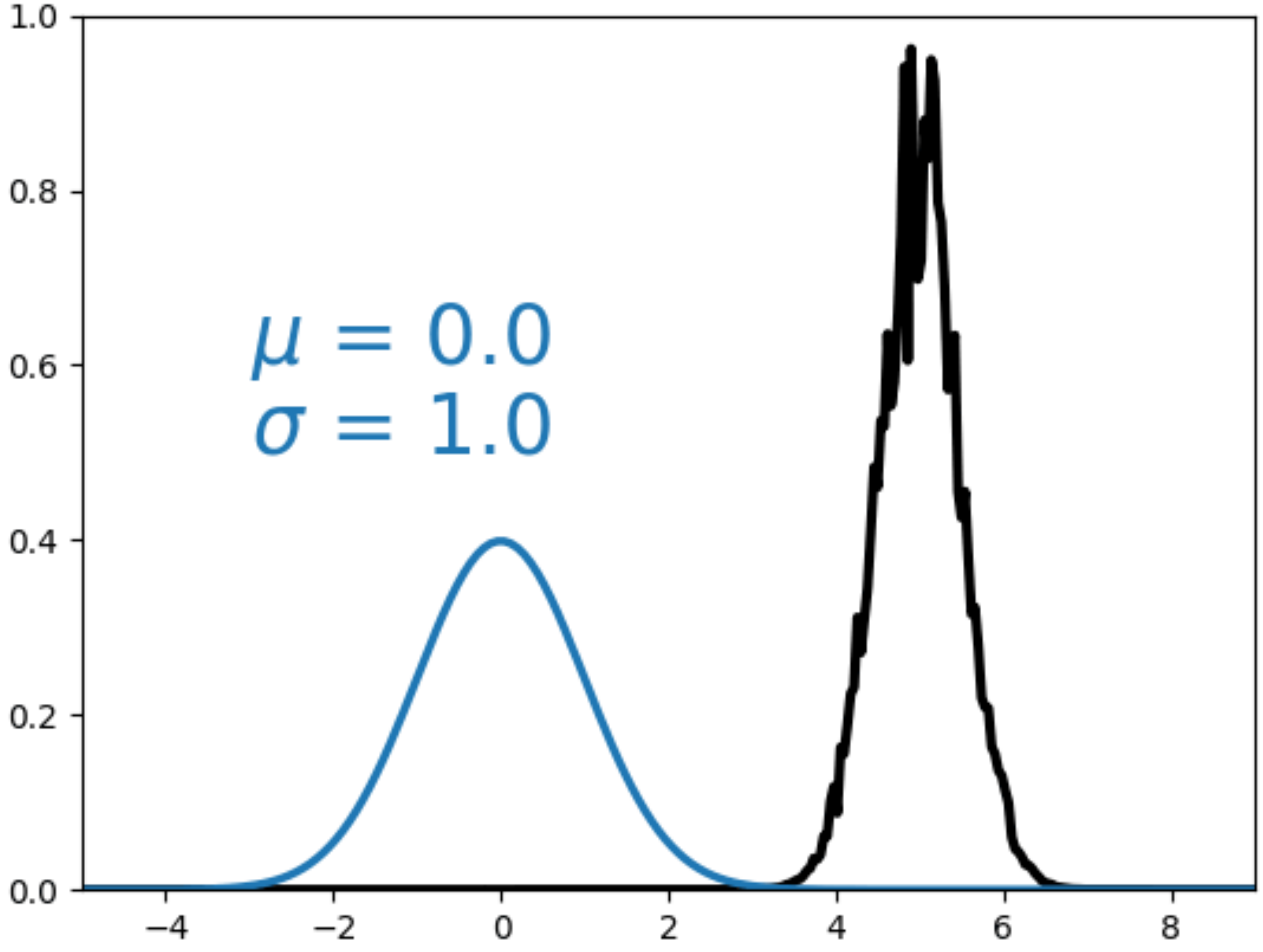


Likelihood $p(x \mid \theta)$ is intractable for ABMs

Proposed solutions include

- Emulation
- Approximate Bayesian Computation
- Neural density ratio estimation

Variational Inference: Bayesian calibration as an optimisation problem



1. Assume posterior can be approximated by a family of distributions

2. Optimise for optimal parameters

Generalized Variational Inference (GVI)

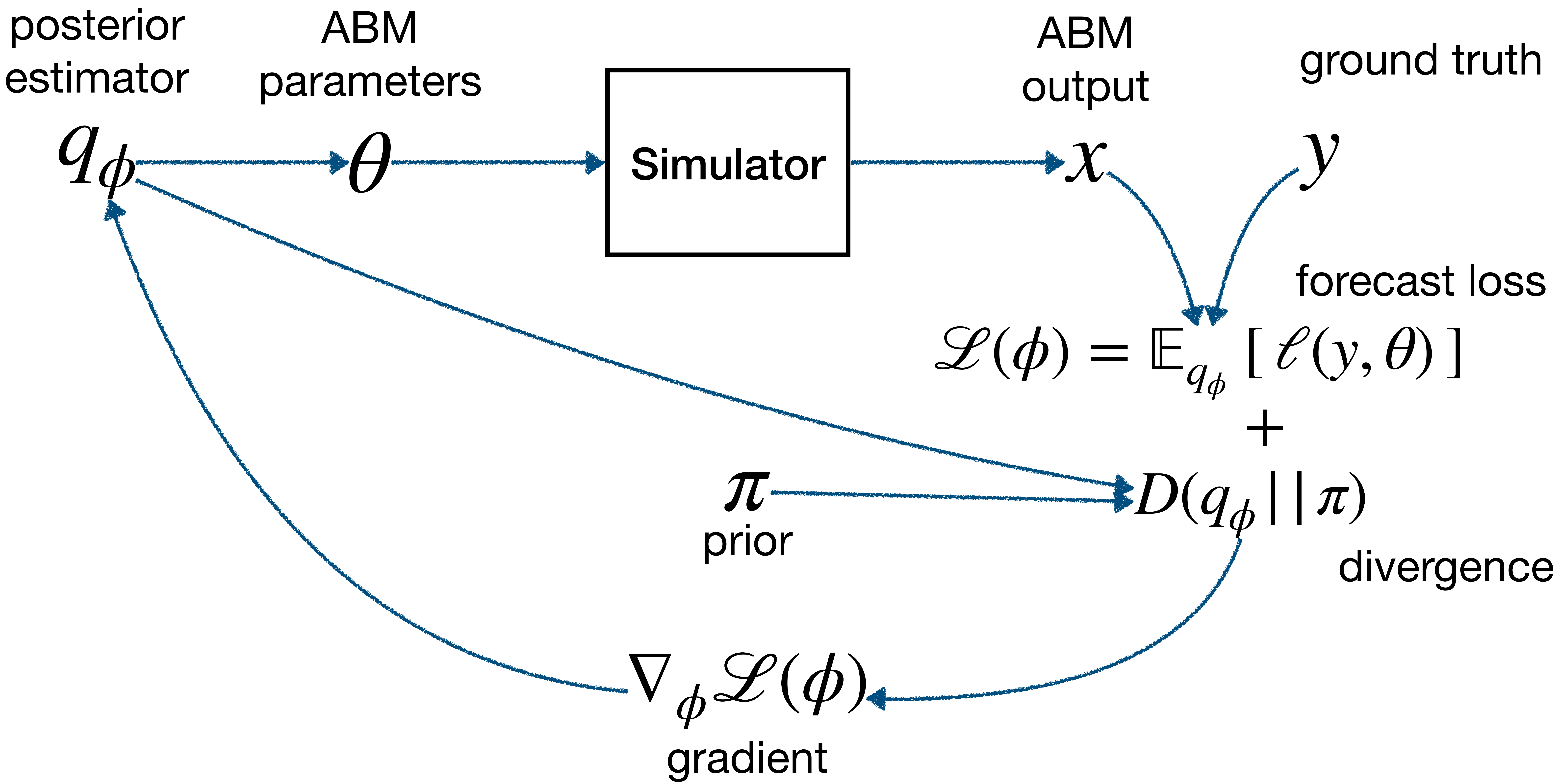
Knoblauch et al., (2022)

Target optimization to **generalised posterior**

↓

More robust to model miss-specification than classical posterior

Generalised Variational Inference



Gradients: path-wise vs score

- Gradient-assisted calibration algorithms need

$$\underbrace{\nabla_\phi \mathbb{E}_{p(\theta\,;\,\phi)}}_{\text{posterior estimator}} \underbrace{\left[f(\theta) \right]}_{\text{simulator}}$$

- Two ways of obtaining the gradient:

1. Differentiating the measure (**score-based gradient**)
2. Differentiating the simulator (**path-wise gradient**)

Differentiable simulators

- Leverage Automatic Differentiation to build simulators
- Use “reparameterisation” techniques to differentiate through randomness.

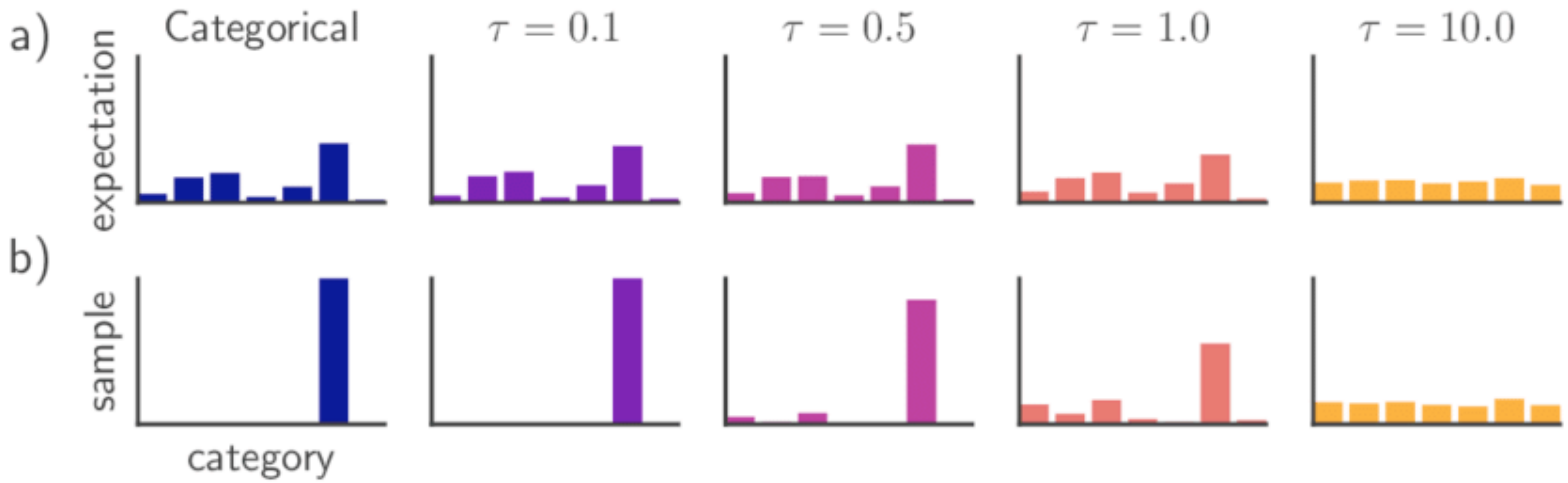
$$x \sim \mathcal{N}(\mu, \sigma) \quad \Longleftrightarrow \quad x = \mu + \sigma\, r \quad r \sim \mathcal{N}(0,1)$$

$$\frac{\mathrm{d}x}{\mathrm{d}\mu} = 1 \quad \frac{\mathrm{d}x}{\mathrm{d}\sigma} = r$$

Differentiable ABMs

The problem of discrete randomness

- Discrete sampling + flow control = no differentiability?
    - Gumbel-Softmax



Jang et al. (2016)

Differentiable Agent-Based Epidemiology

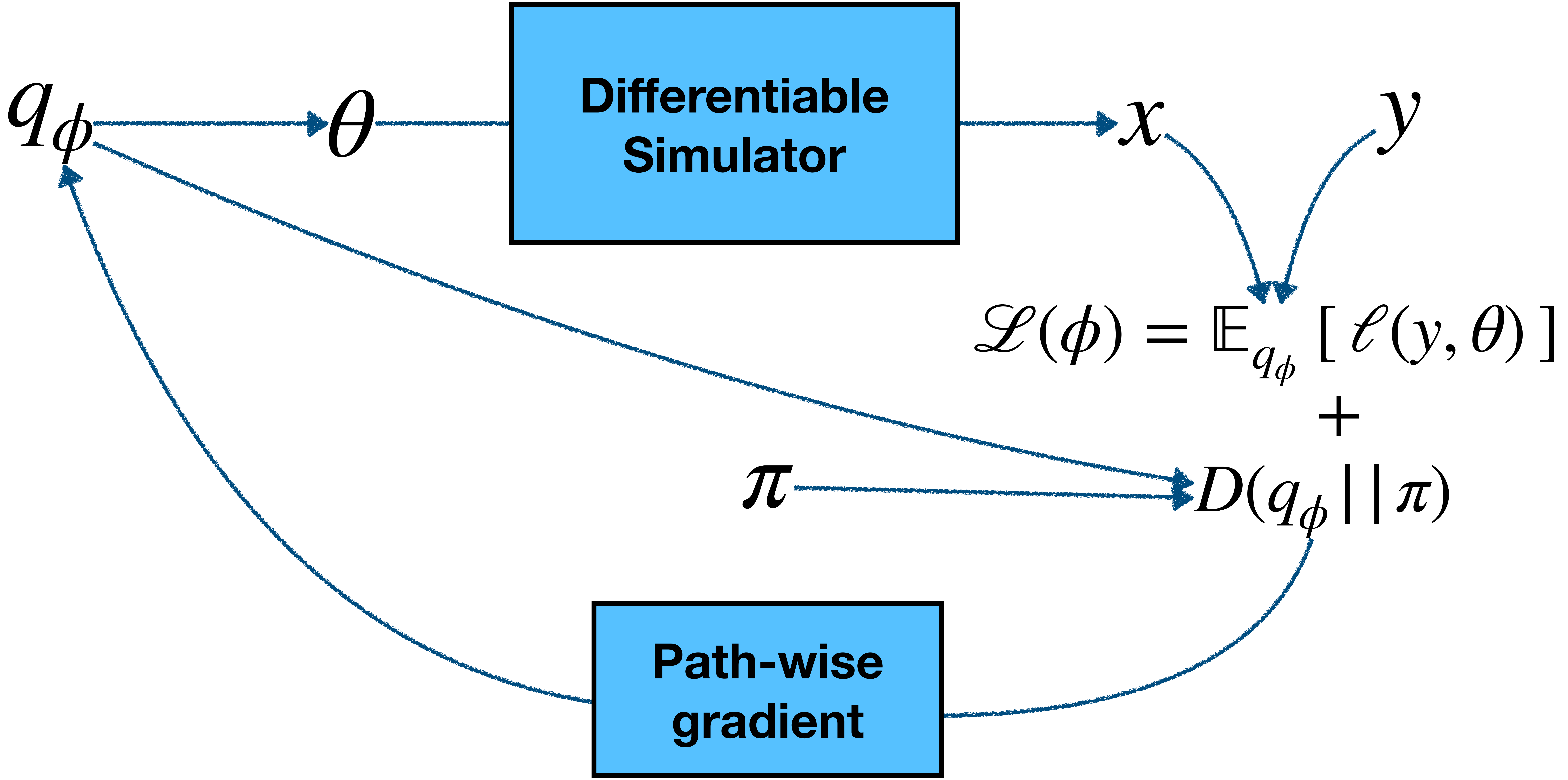
Chopra et al. (2023), Quera-Bofarull et al. (2023)

JUNE model
8 M agents (London)

	Simulation	Calibration	Sensitivity Analysis
JUNE	50 hours	100k hours	5k hours
GradABM-June (CPU)	5 minutes	10 hours	10 minutes
GradABM-June (GPU)	5 seconds	20 minutes	10 seconds

x40,000 speed-up !

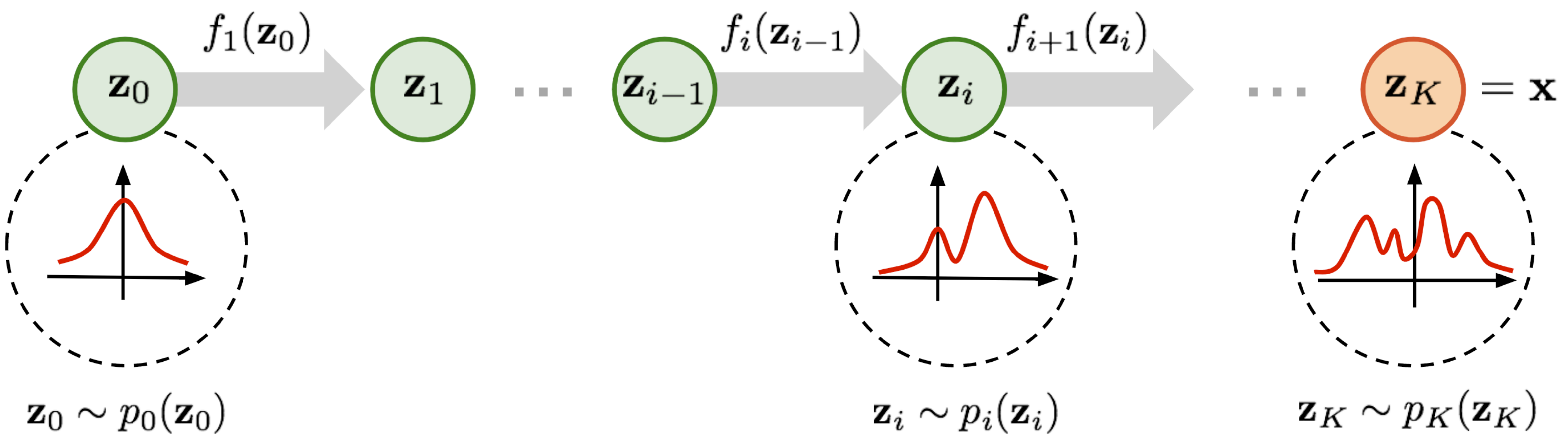
Bayesian Inference for Differentiable Simulators (BIRDS)

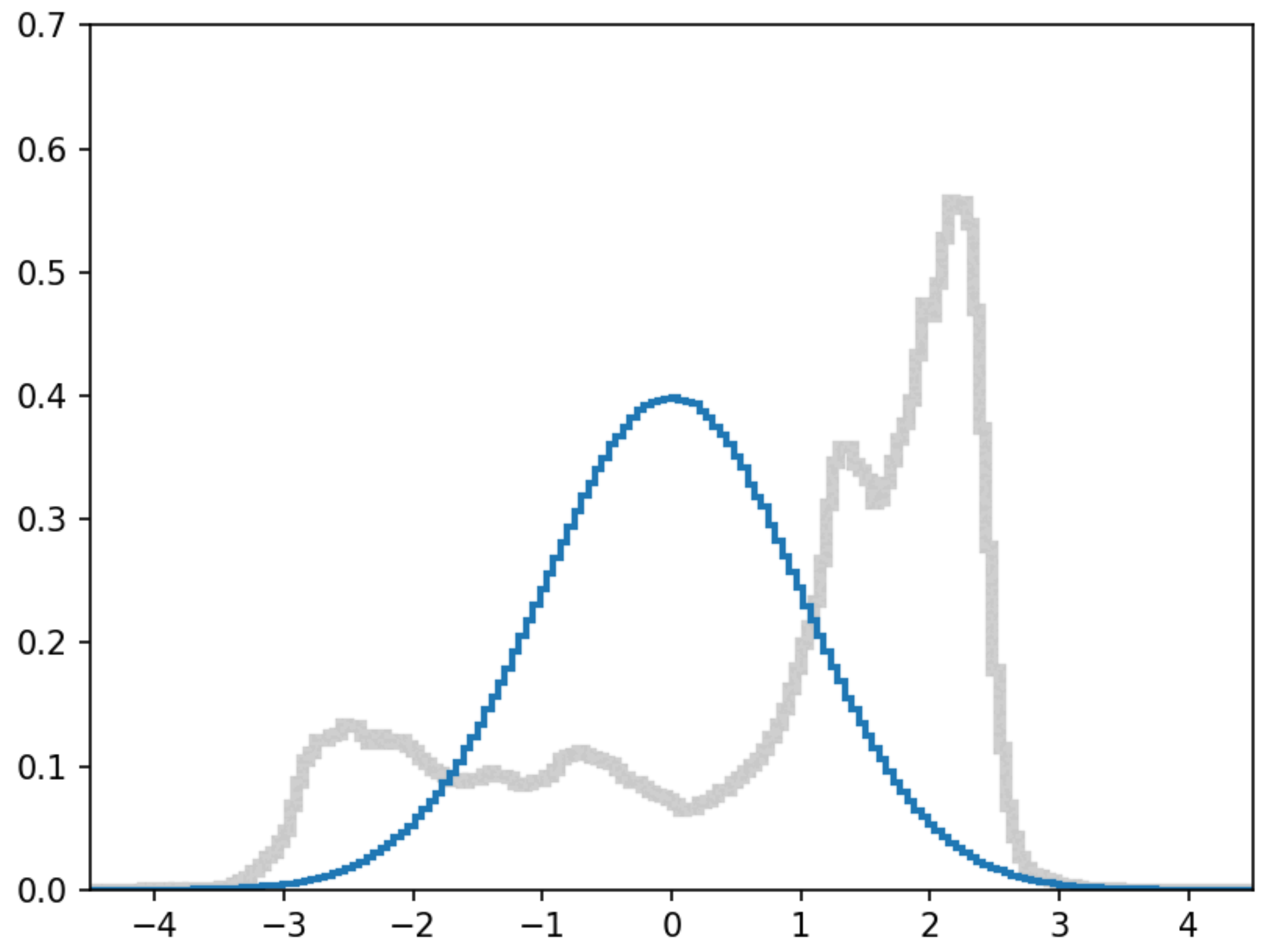


Normalizing Flows

What do we choose for q?

Image credit: Lilian Weng





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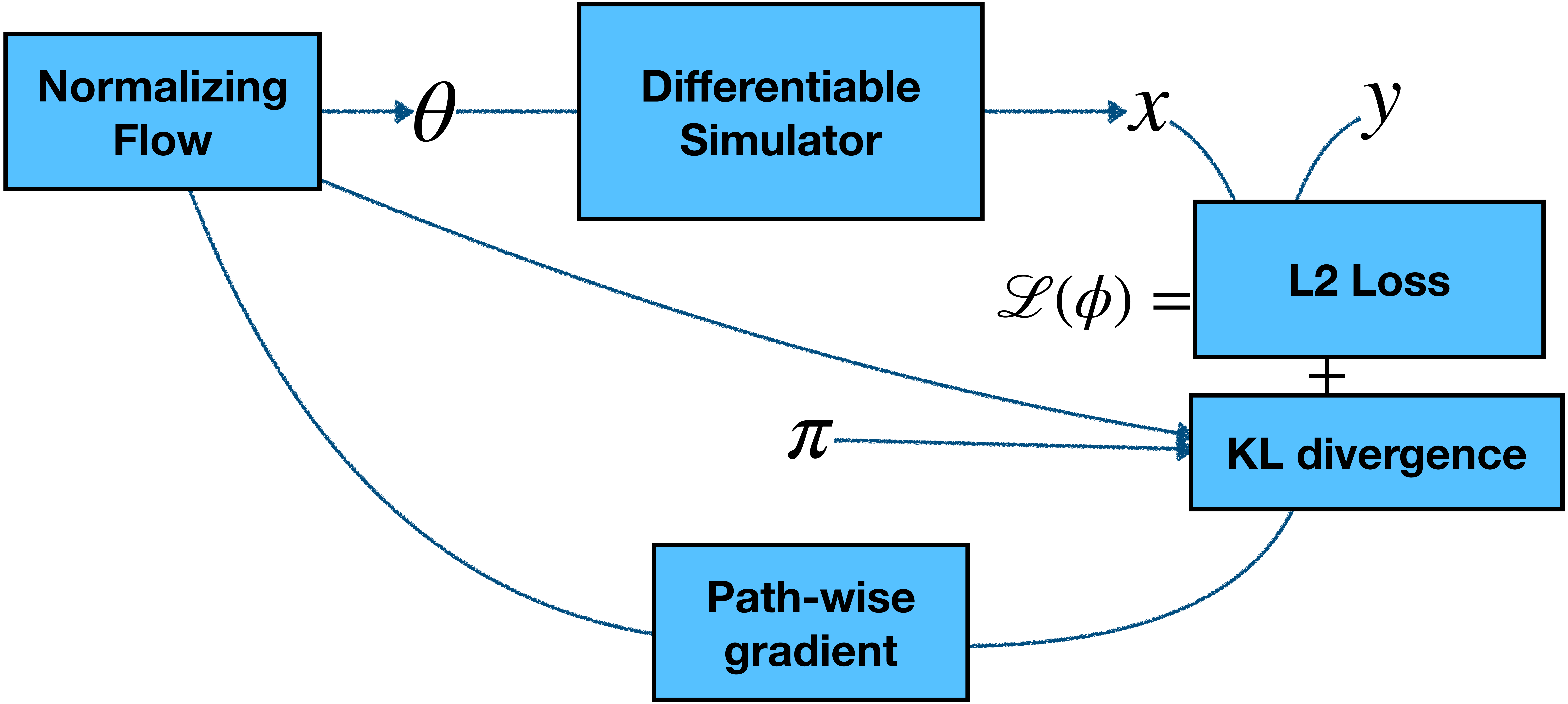
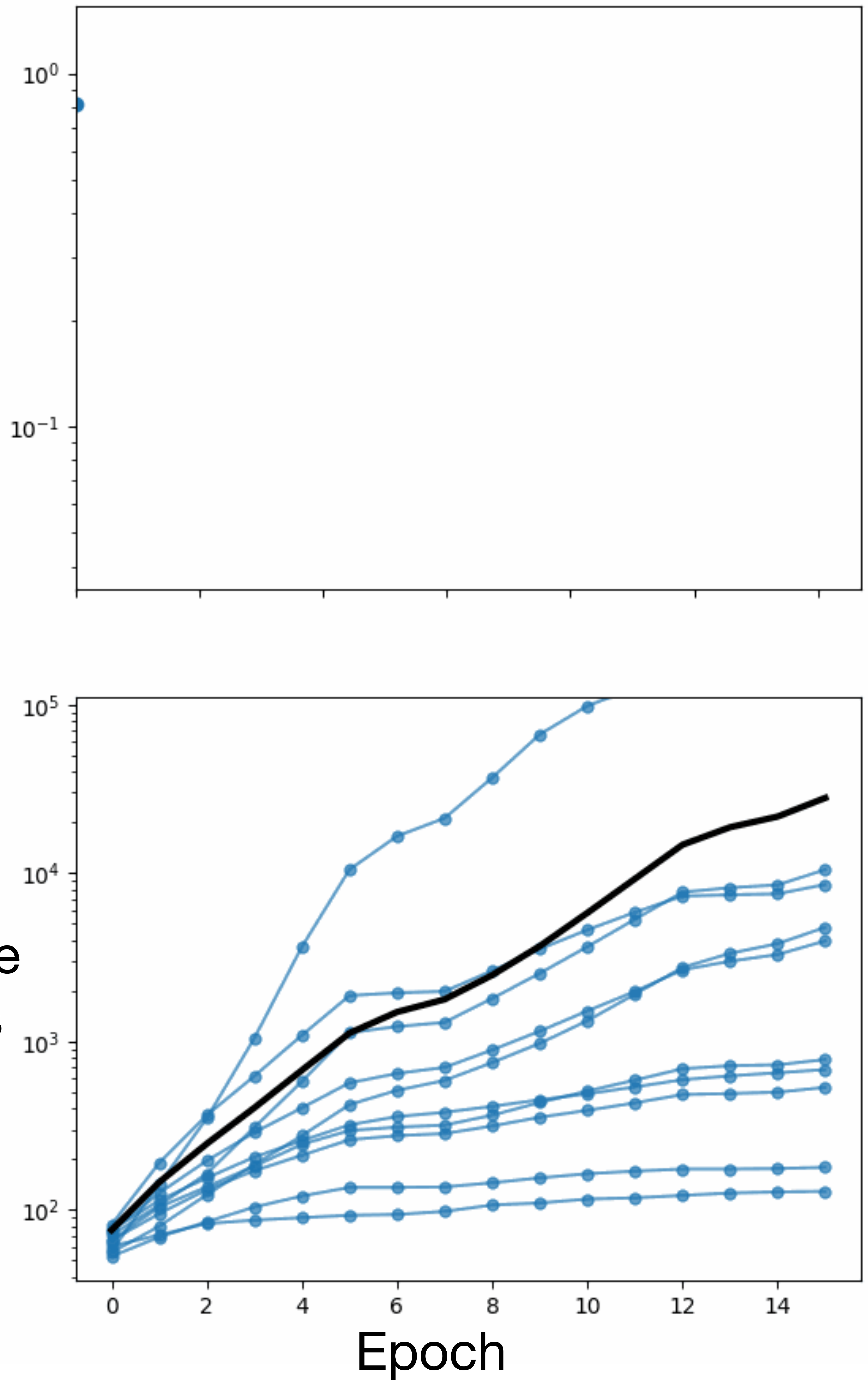


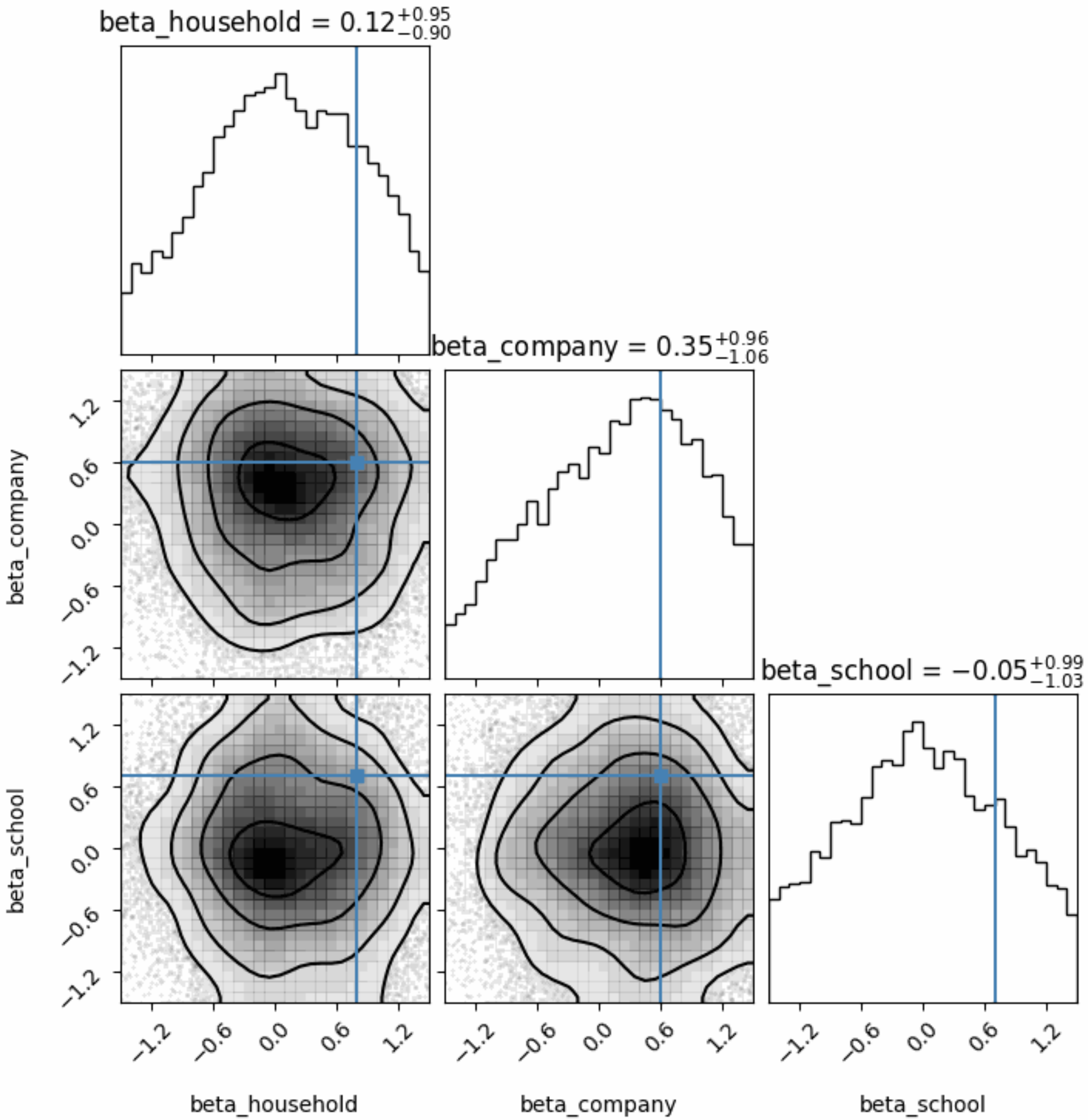
Experiment with JUNE

- ABM model of Covid19
- Model
  - ~200k agents
  - 3 layers of interactions (household, company, school)
  - Calibrate to synthetic data

Loss

Cumulative Infections





Conclusions

1. Bayesian approaches to calibrating ABMs have numerous benefits

2. ABMs can be made differentiable even with discrete randomness and control flow

3. Diff simulators + Bayesian inference (via Normalizing Flows) promising route to calibrate large-scale ABMs efficiently

Paper + slides: www.arnau.ai/iclr