Bayesian calibration of differentiable agent-based models

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AI4ABM workshop — ICLR 2023

Calibration of ABMs

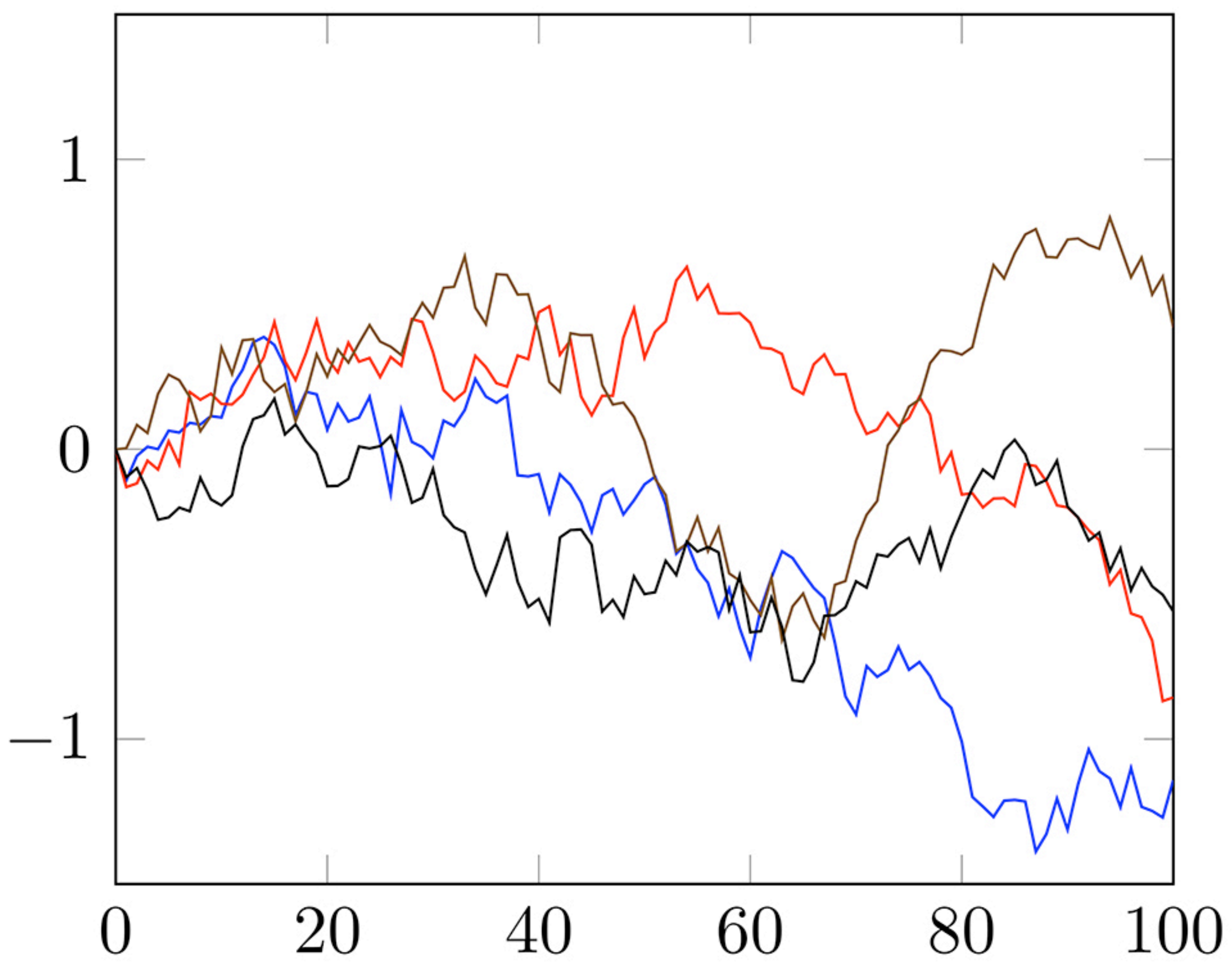
- Forward simulation:

θ

ABM parameters

ABM simulator

x



ABM calibration aims to inverse this process

Calibration of ABMs

$$\theta \longrightarrow \boxed{\text{Simulator}} \longrightarrow x$$

$$x \longrightarrow \boxed{\text{Calibrator}} \longrightarrow \theta$$

Why is it hard?

- Expensive simulator

+

- Large parameter space

Calibration of ABMs

Bayesian calibration

Ideally, we want to get all θ that can create *x*

[TODO: June example of infections in schools vs companies for 1st wave…]

The object of interest is the **Bayesian posterior**: $p(\theta | x)$

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

Bayesian calibration

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

likelihood

prior

ABMs have computationally intractable likelihoods

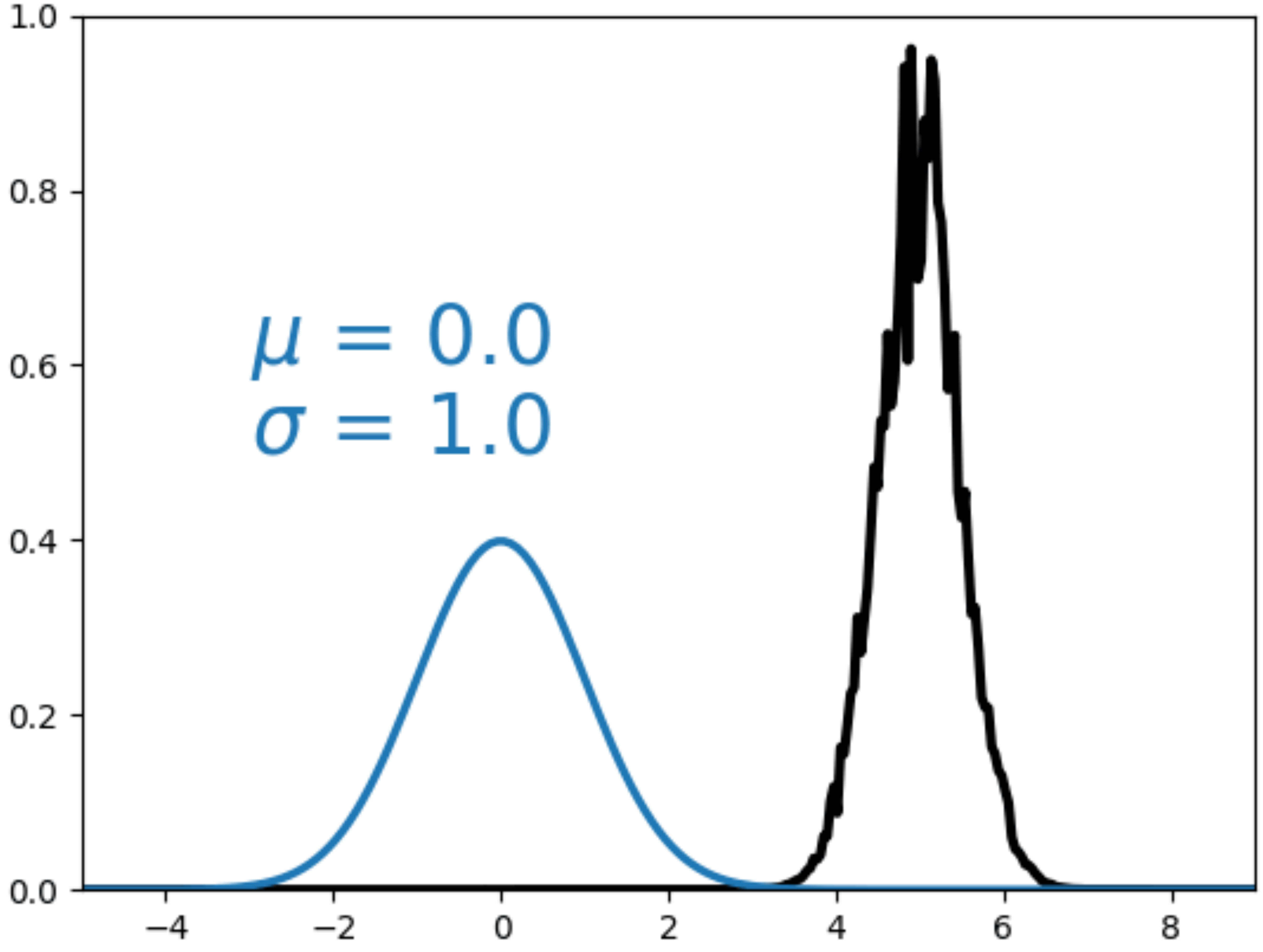
Proposed solutions include

Emulation

Approximate Bayesian Computation

Neural density ratio estimation

Bayesian calibration as an optimisation problem (variational inference)



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

2. Optimise for optimal parameters

Generalized Variational Inference (GVI)

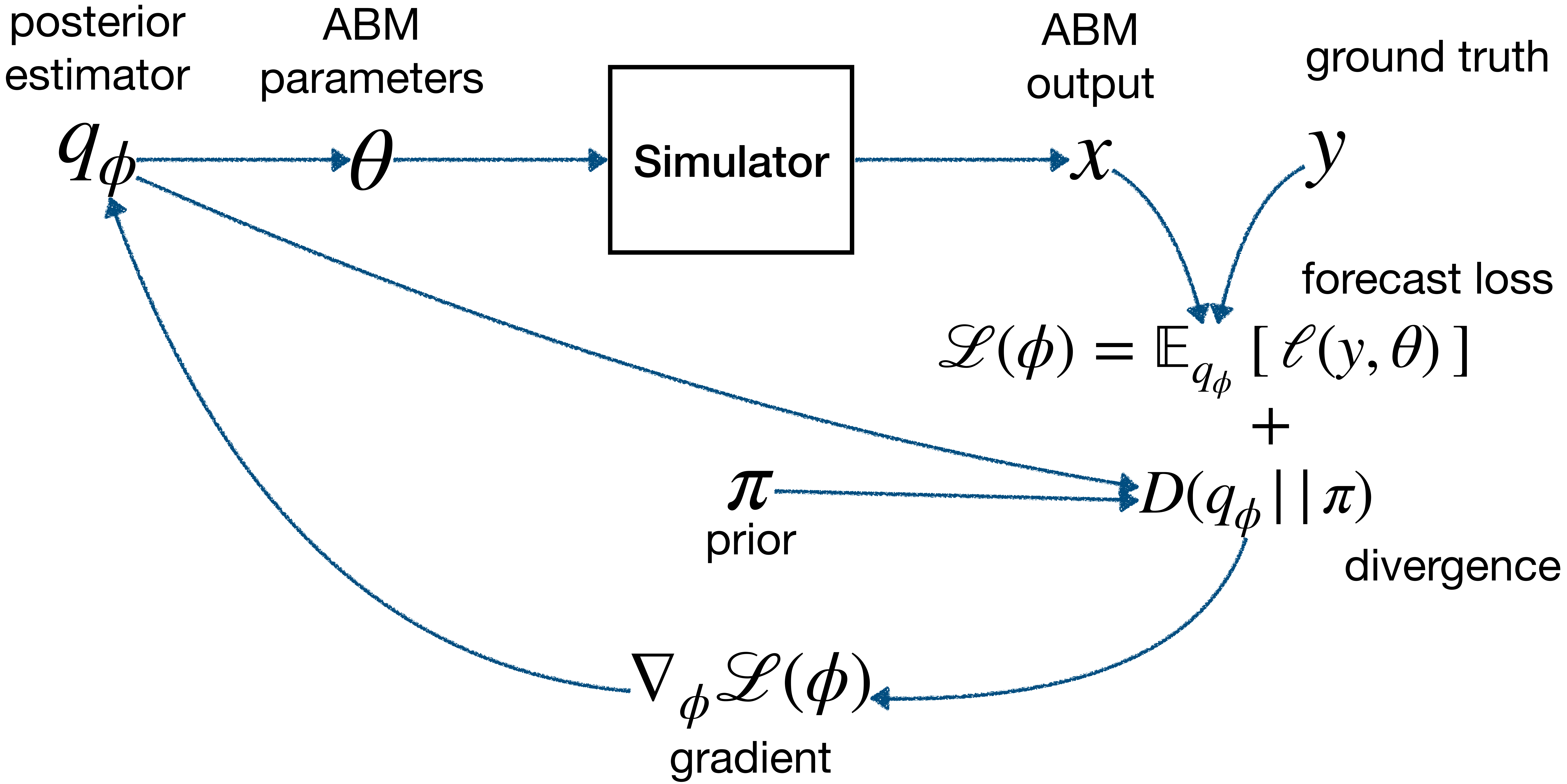
Knoblauch et al., (2022)

- [TODO: Ask Joel about what details to put here…) hard to summarize

- Generalized posteriors -> More robust to miss-specification

- Use VI to approximate the generalized posterior.

Generalised Variational Inference



Gradients: path-wise vs score

- Gradient-assisted calibration algorithms need

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

posterior estimator

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.

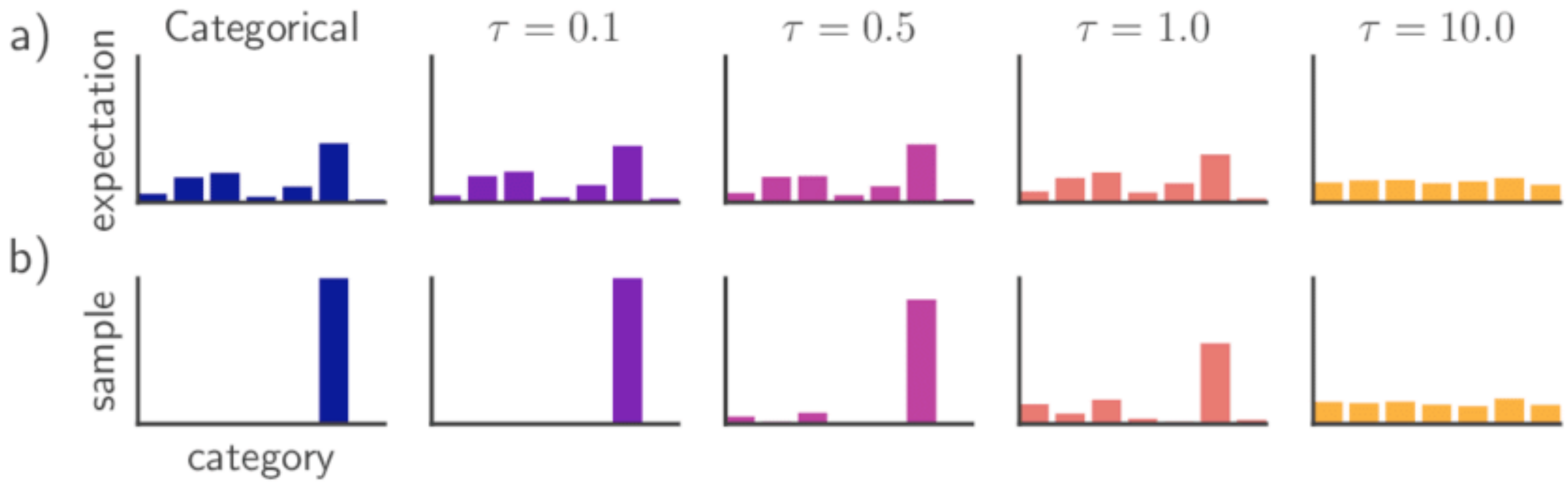
$$x \sim \mathcal{N}(\mu, \sigma) \iff x = \mu + \sigma r \quad r \sim \mathcal{N}(0,1)$$

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

Differentiable ABMs

The problem of discrete randomness

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



Jang et al. (2016)

Differentiable Agent-Based Epidemiology

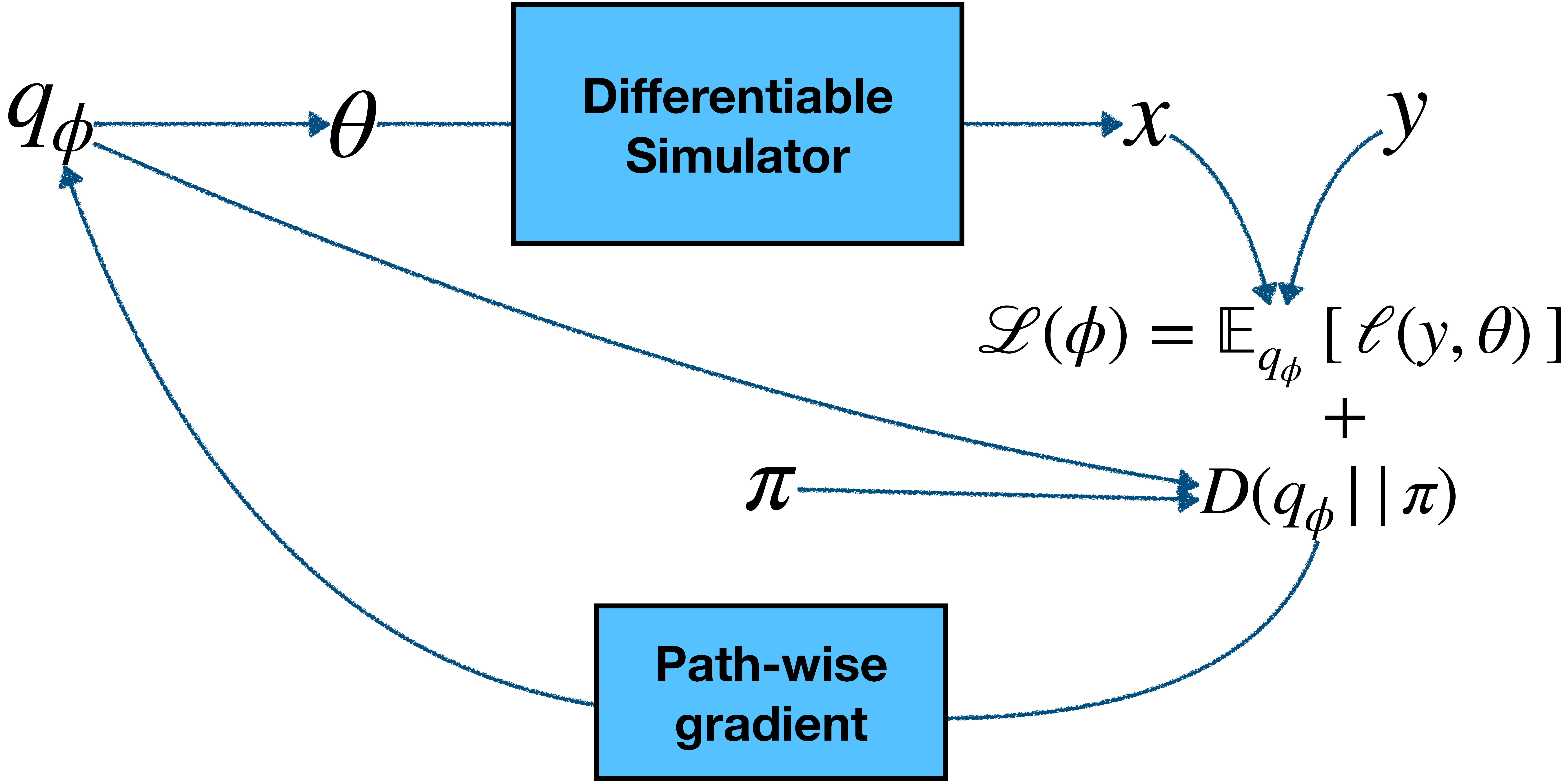
Chopra et al. (2023), Quera-Bofarull et al. (2023)

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 !

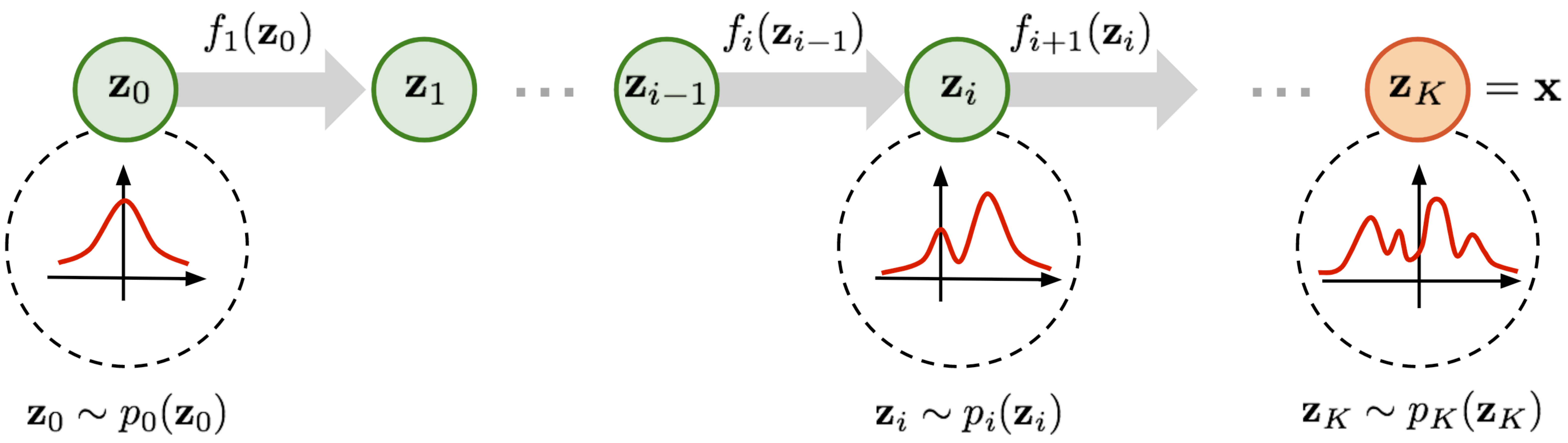
Bayesian Inference for Differentiable Simulators (BIRDS)

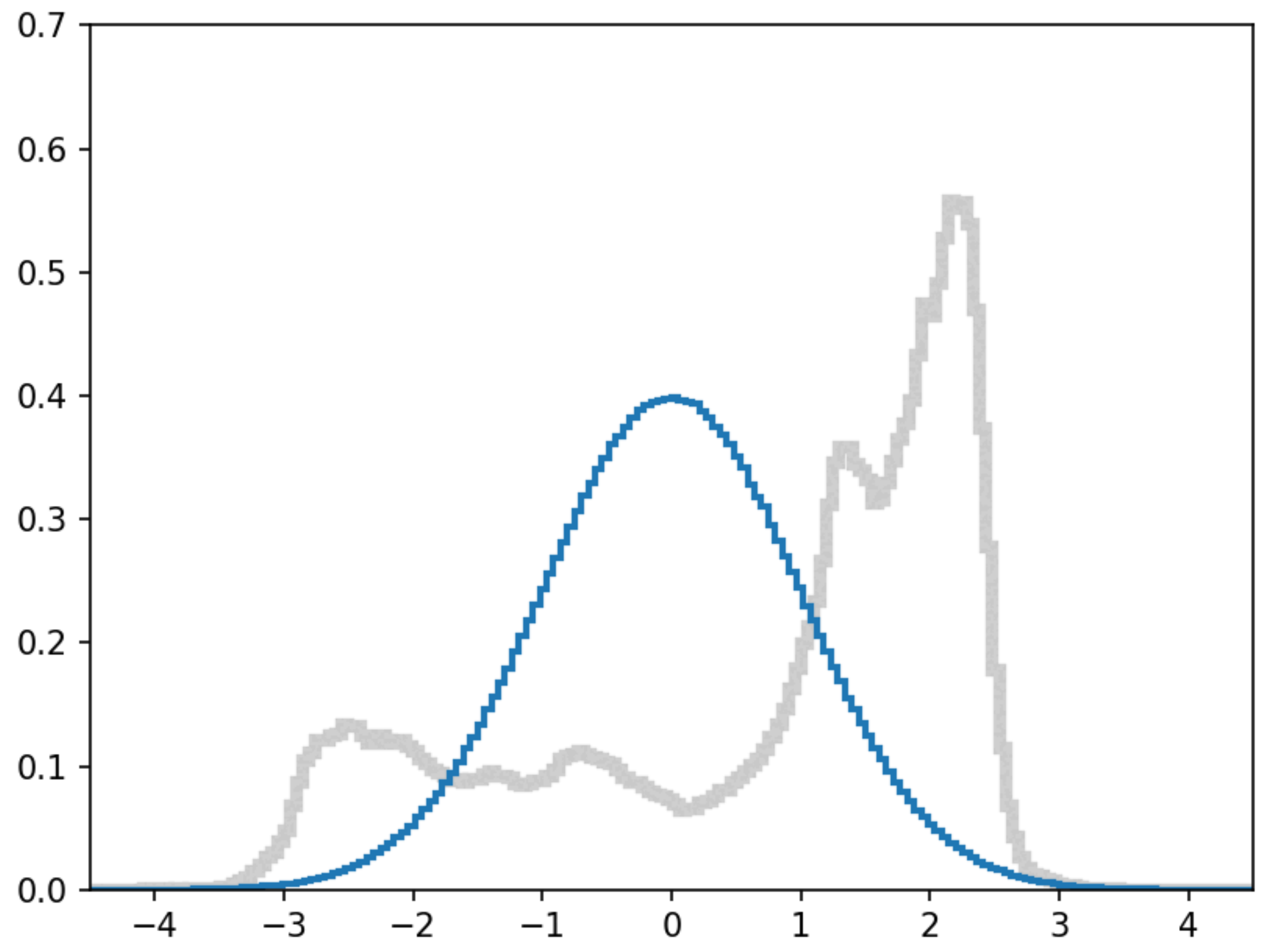


Normalizing Flows

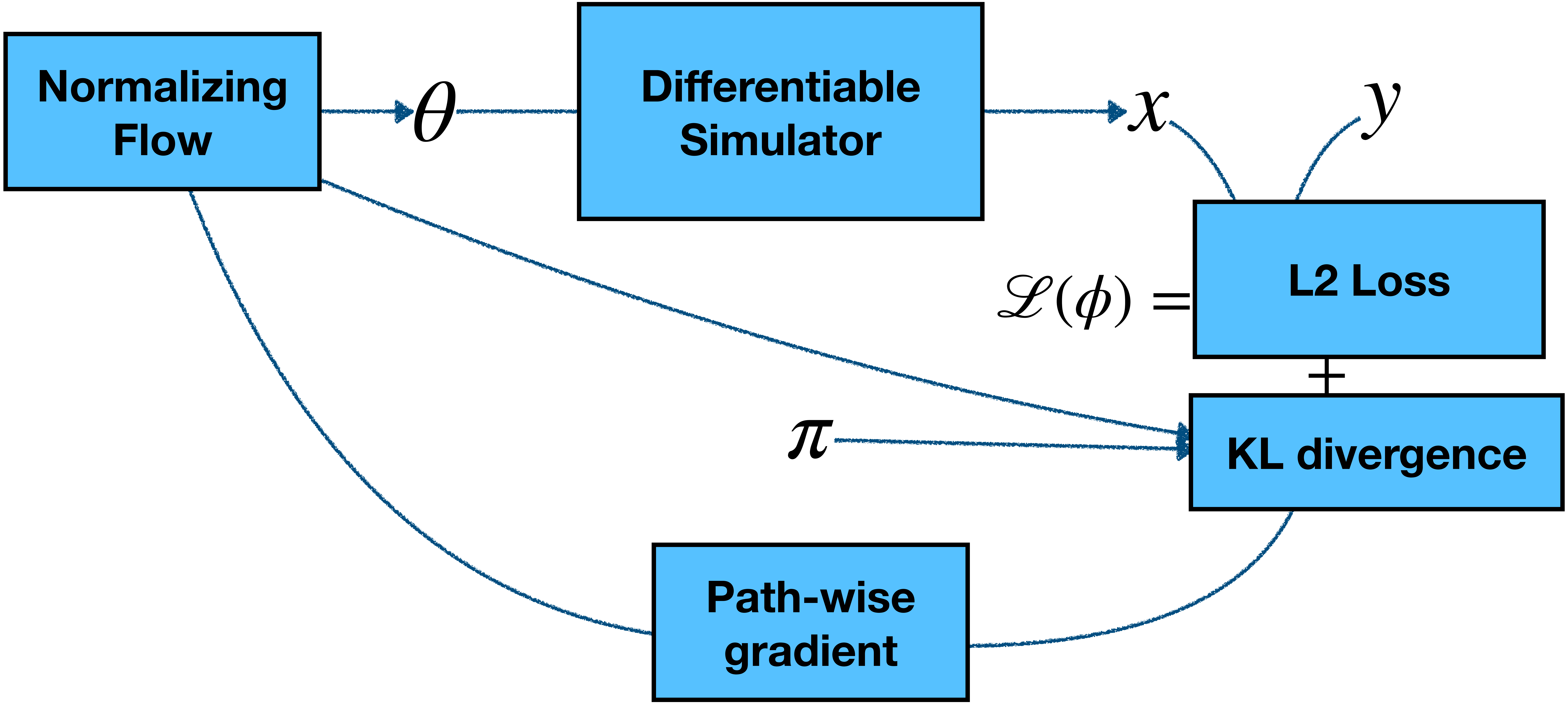
What do we choose for q?

Image credit: Lilian Weng



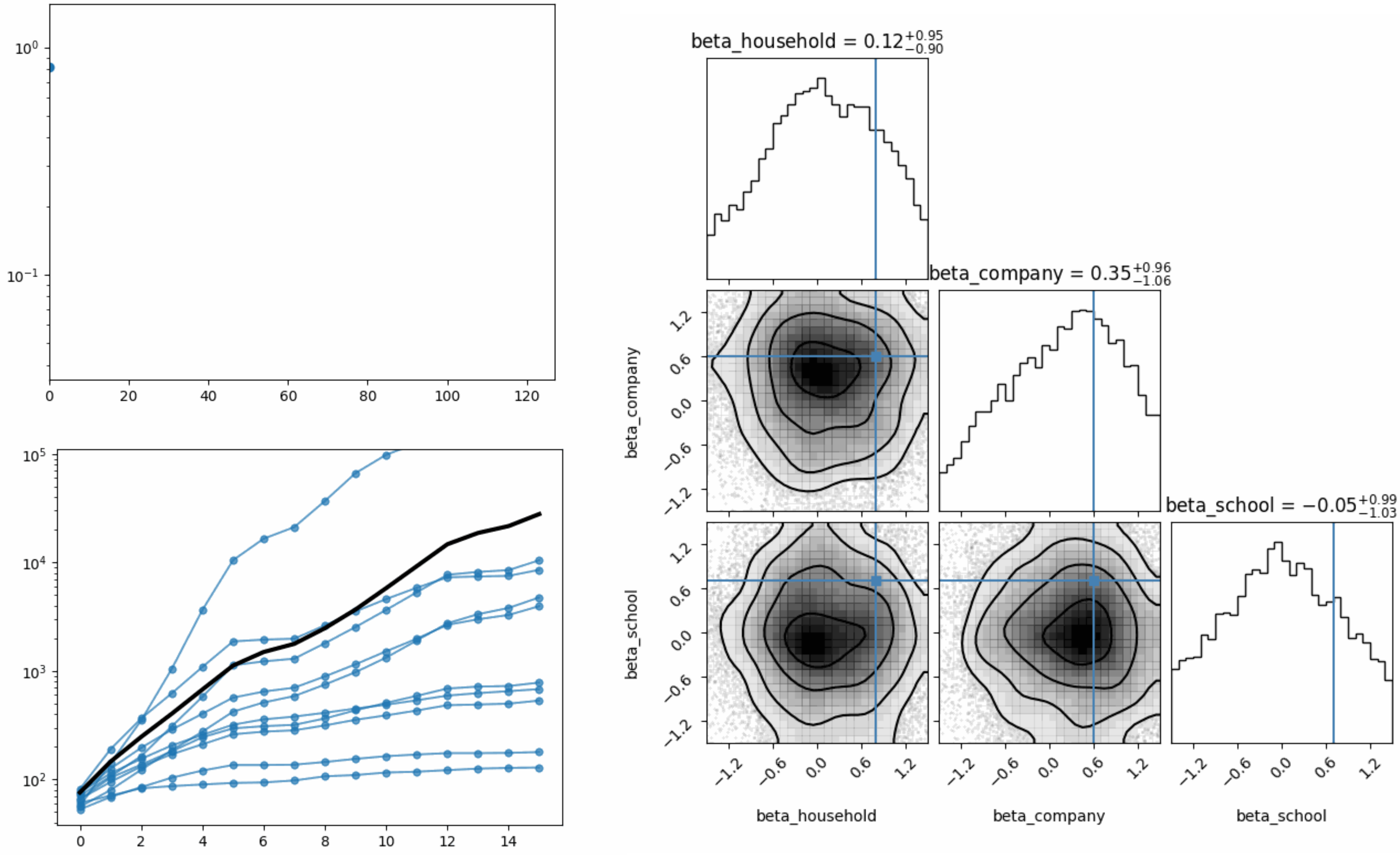


Bayesian Inference for Differentiable Simulators (BIRDS)



Experiment with JUNE

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


beta_household = $0.12^{+0.95}_{-0.90}$
beta_company = $0.35^{+0.96}_{-1.06}$
beta_school = $-0.05^{+0.99}_{-1.03}$
beta_company
beta_school
beta_household
beta_company
beta_school

Conclusions

1. **ABM calibration should be Bayesian**

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