Does Bayes have to be slow?

A glimpse into amortized Bayesian inference

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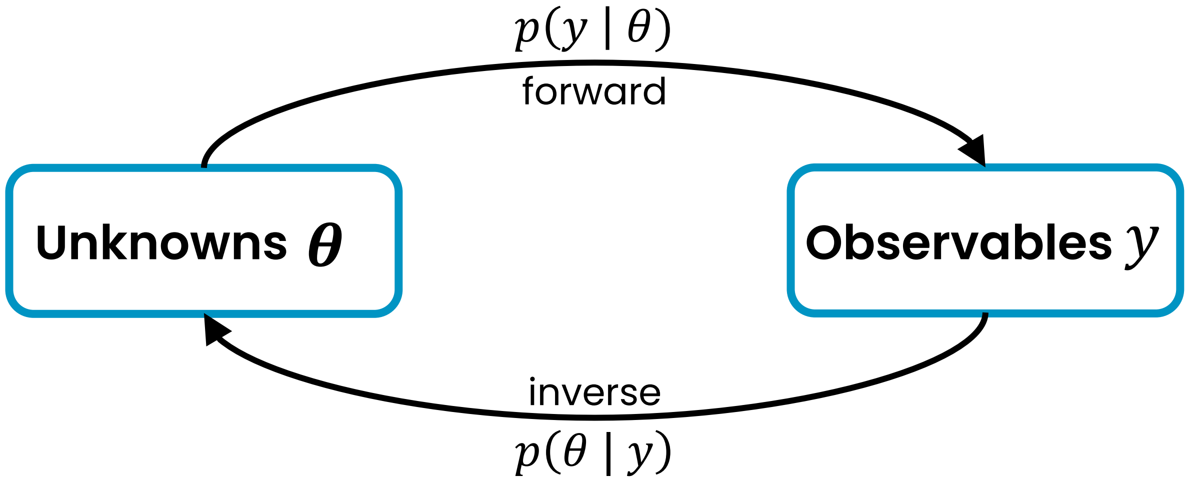
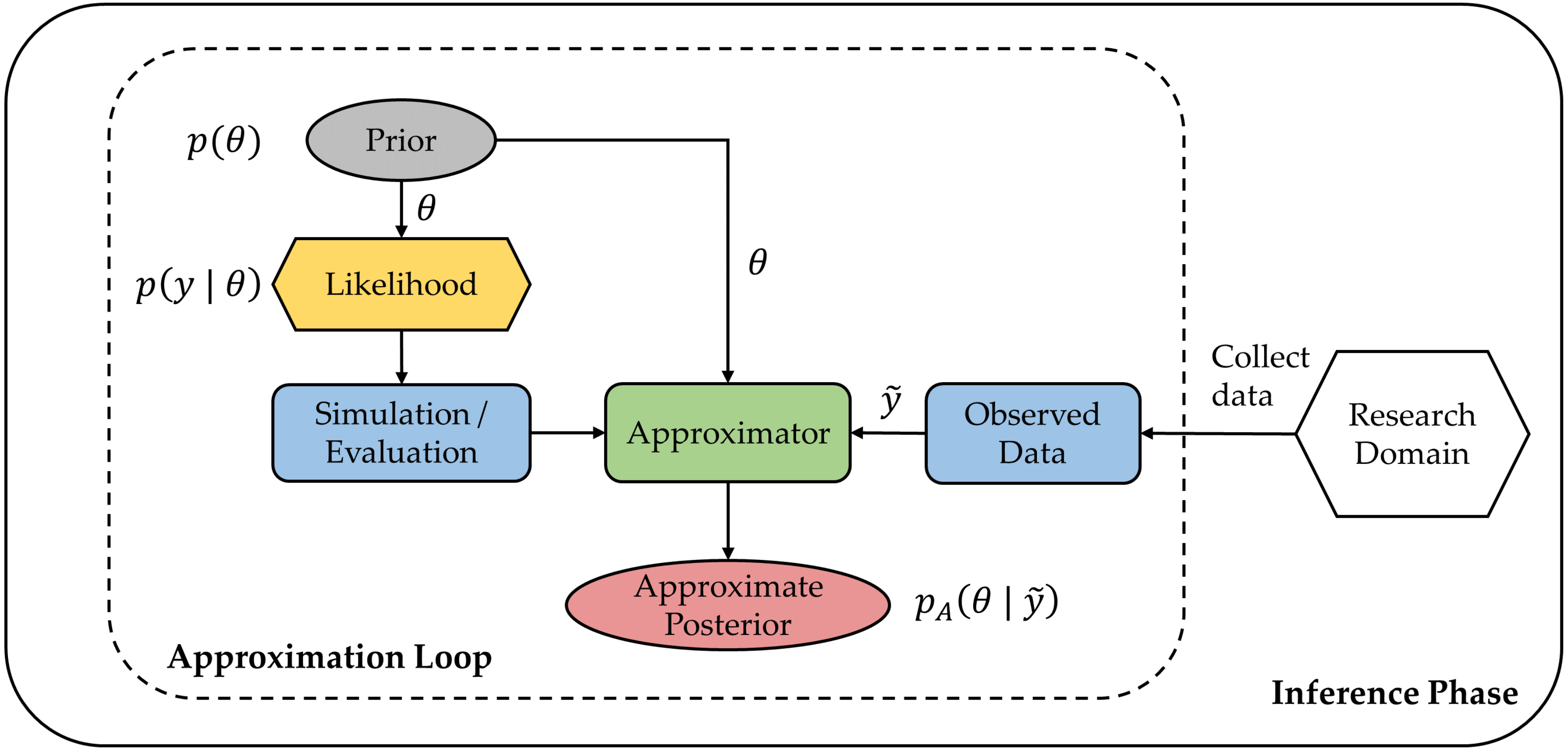
Inverse Problems



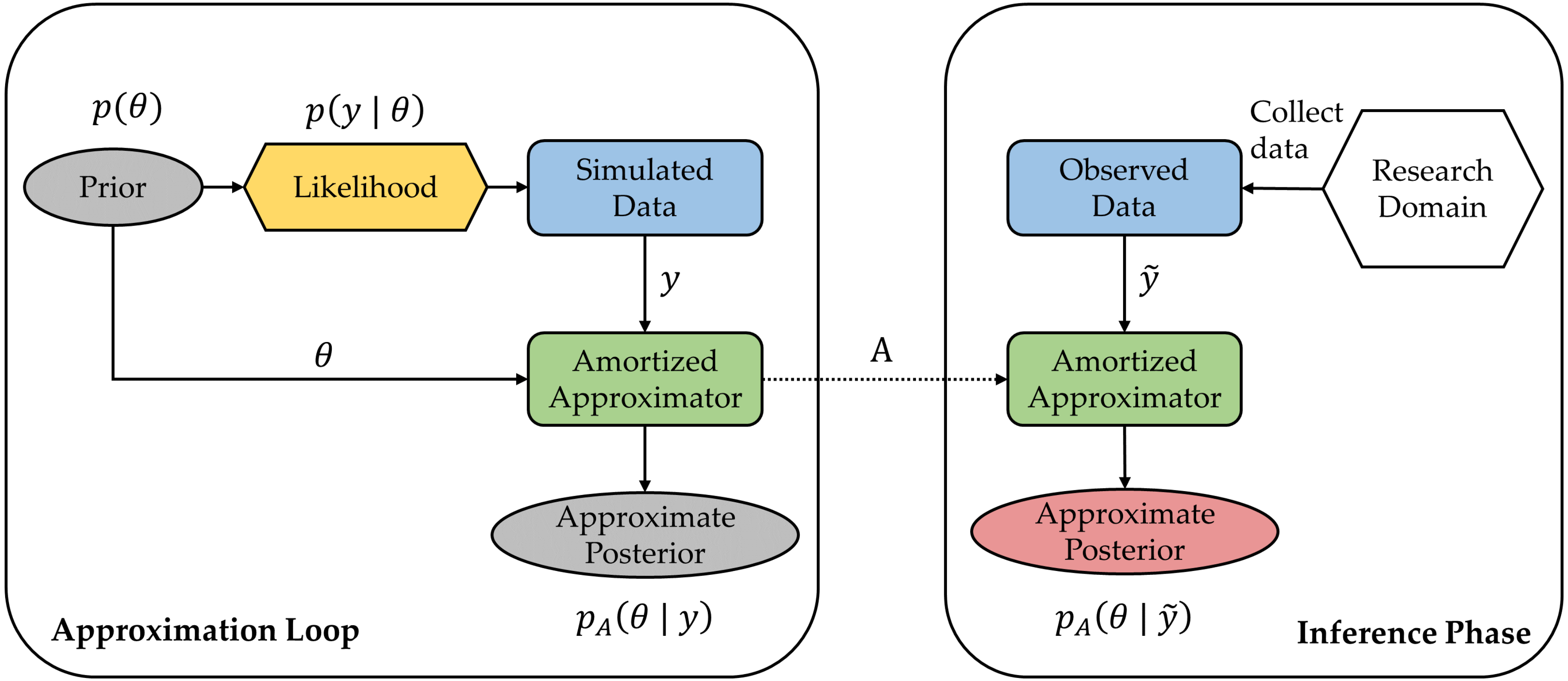
Statistical modeling:	**Parameters $\boldsymbol{\theta}$**	**Data $\boldsymbol{y}$**
Epidemiology:	Virus attributes	Infection curve (time series)
Image processing:	Crisp image	Blurry image
Psychology:	Cognitive parameters	Reaction times

Non-amortized Bayesian inference



Approximation and inference are **coupled**. No resource pooling.

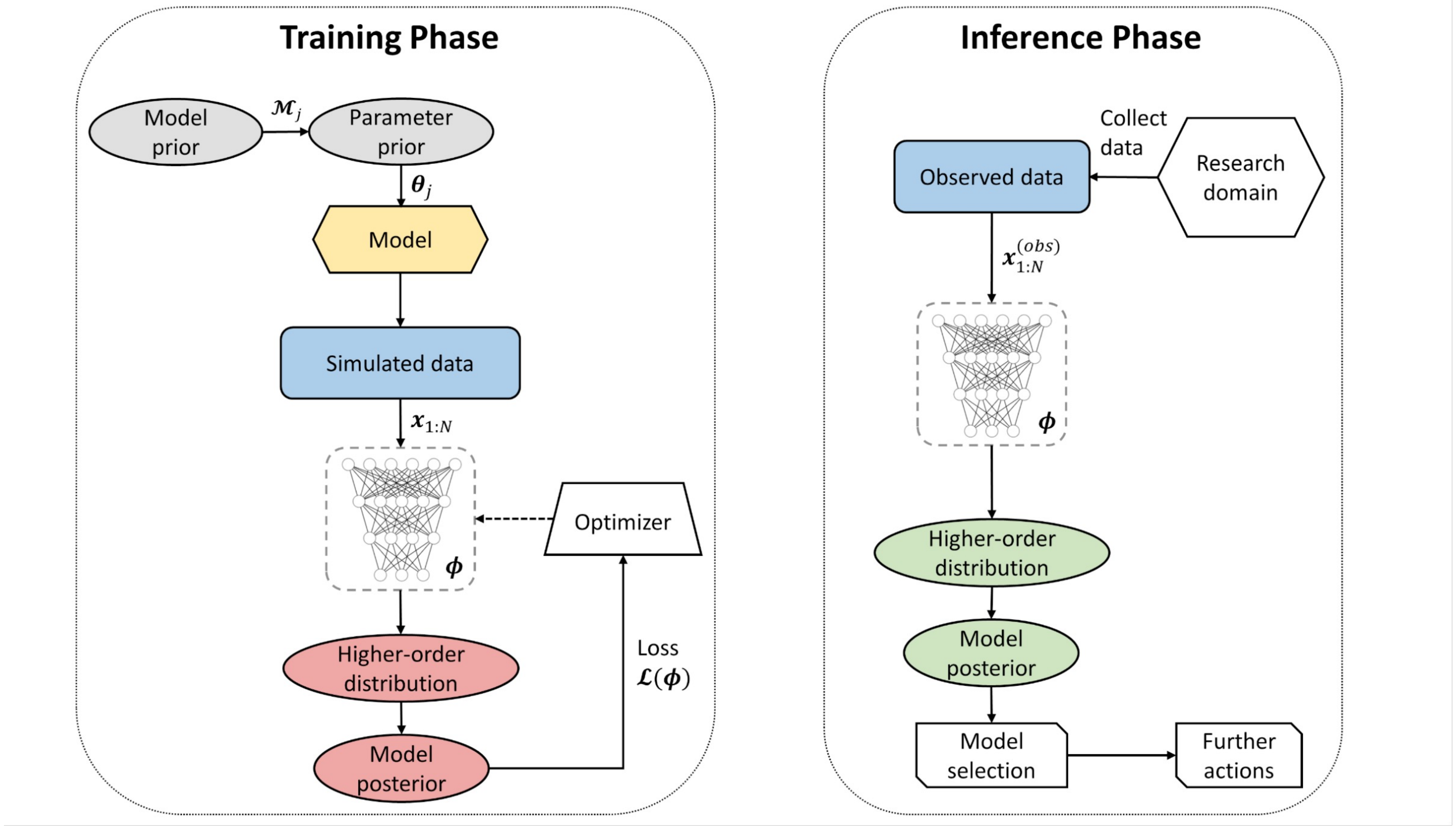
Amortized Bayesian inference (ABI)



Approximation and inference are **decoupled**. Pooling of resources.

https://arxiv.org/abs/2209.02439

Amortized Model Comparison



https://arxiv.org/abs/2004.10629

Loss Functions: Variational Inference

<u>Backward KL divergence</u>

$$\text{minimize} \quad KL(p_A(\theta \mid \tilde{y}) \,||\, p(\theta \mid \tilde{y})) = \int \log\left(\frac{p_A(\theta \mid \tilde{y})}{p(\theta \mid \tilde{y})}\right) p_A(\theta \mid \tilde{y})\, d\theta$$

$$\Longleftrightarrow \quad \text{maximize} \quad \frac{1}{S}\sum_{s=1}^{S} \log\left(\frac{p(\theta^{(s)}, \tilde{y})}{p_A(\theta^{(s)} \mid \tilde{y})}\right) \quad \text{for} \quad \theta^{(s)} \sim p_A(\theta \mid \tilde{y})$$

The ELBO just requires the joint density of the model

Loss Functions: Simulation-Based Inference

Forward KL divergence

$$\text{minimize} \quad KL(p(\theta \mid \tilde{y}) \,||\, p_A(\theta \mid \tilde{y})) = \int \log \left(\frac{p(\theta \mid \tilde{y})}{p_A(\theta \mid \tilde{y})} \right) p(\theta \mid \tilde{y}) \, d\theta$$

$$\iff \quad \text{maximize} \quad \frac{1}{S} \sum_{s=1}^{S} \log p_A(\theta^{(s)} \mid \tilde{y}) \quad \text{for} \quad \boxed{\theta^{(s)} \sim p(\theta \mid \tilde{y})}$$

Minimizing the expected KL over the whole data space

$$\text{minimize} \quad E_{p(y)} \left[KL(p(\theta \mid y) \,||\, p_A(\theta \mid y)) \right]$$

$$\iff \quad \text{maximize} \quad \frac{1}{S} \sum_{s=1}^{S} \log p_A(\theta^{(s)} \mid y^{(s)}) \quad \text{for} \quad \boxed{(\theta^{(s)}, y^{(s)}) \sim p(\theta, y)}$$

How to obtain the posterior approximator?

Sample $z^{(s)} \sim \mathrm{multinormal}(0, I)$

Transform to $\theta^{(s)} = f_\phi(z^{(s)} \mid y)$ with an invertible neural network

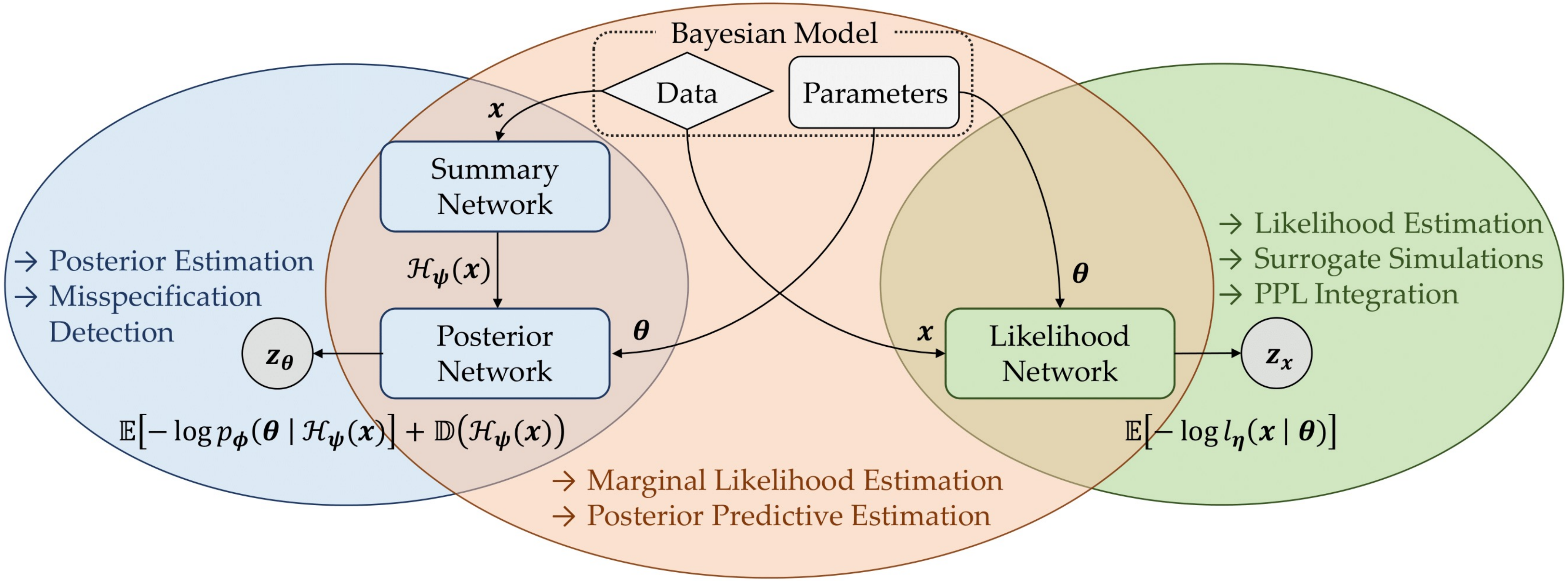
Obtain the approximator's density for training via expected KL divergence:

$$p_A(\theta \mid y) = p(z = f_\phi^{-1}(\theta \mid y)) \left| \det \left(\frac{\delta f_\phi^{-1}(\theta \mid y)}{\delta \theta} \right) \right|$$

https://arxiv.org/abs/2003.06281

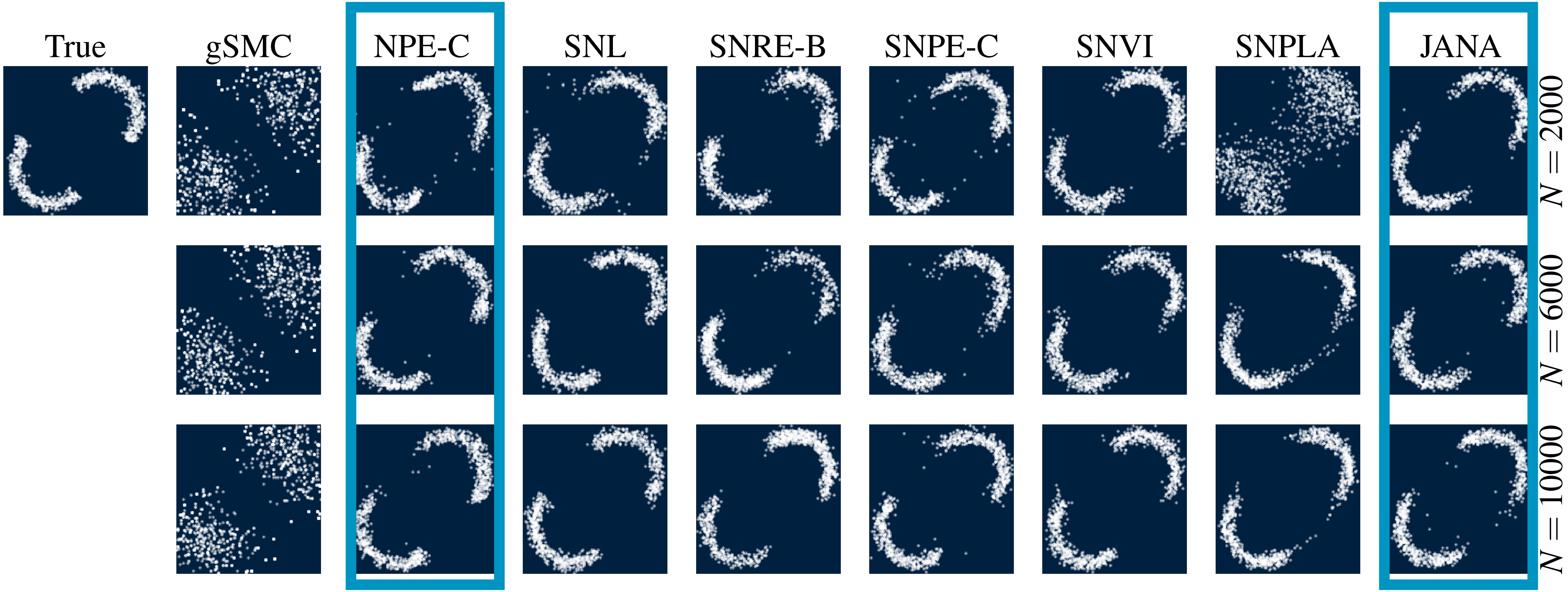
Jointly amortized learning

- Jointly amortized neural approximation (JANA)



https://arxiv.org/abs/2302.09125

Isn't amortized inference wasteful?



Amortized methods perform on-par with non-amortized counterparts

https://arxiv.org/abs/2302.09125

Potential of Amortized Bayesian Inference

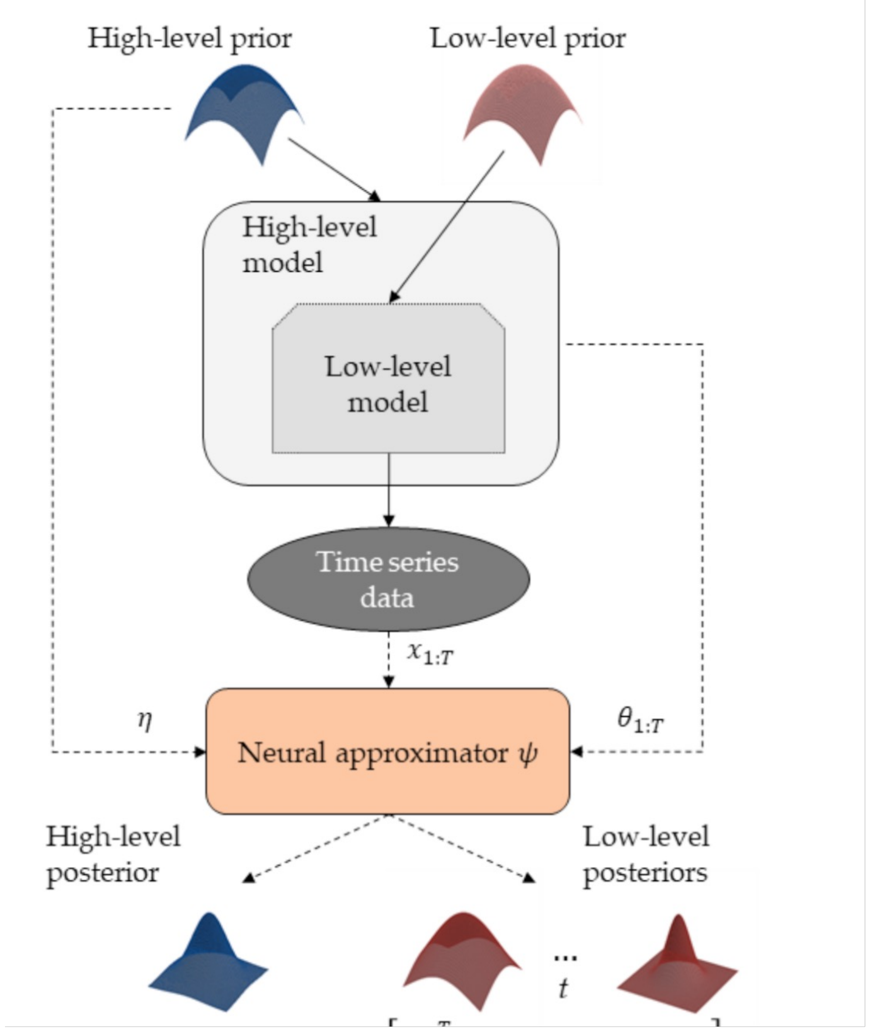
Massive number of inference repetitions

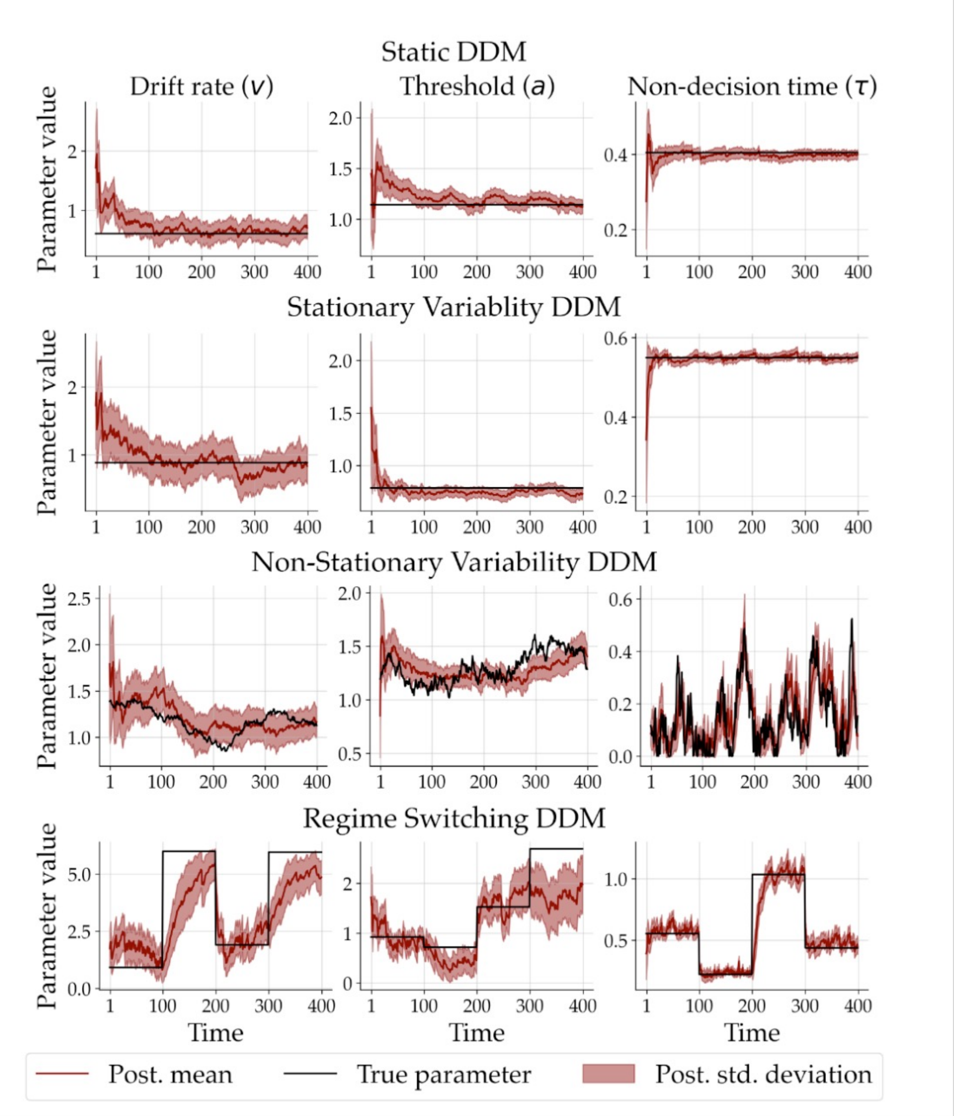
- Many data sets
- Cross-validation
- Sensitivity analyses, multiverse analyses

Real-time inference

- Neurological monitoring
- Adaptive experimental design
- Disease surveillance

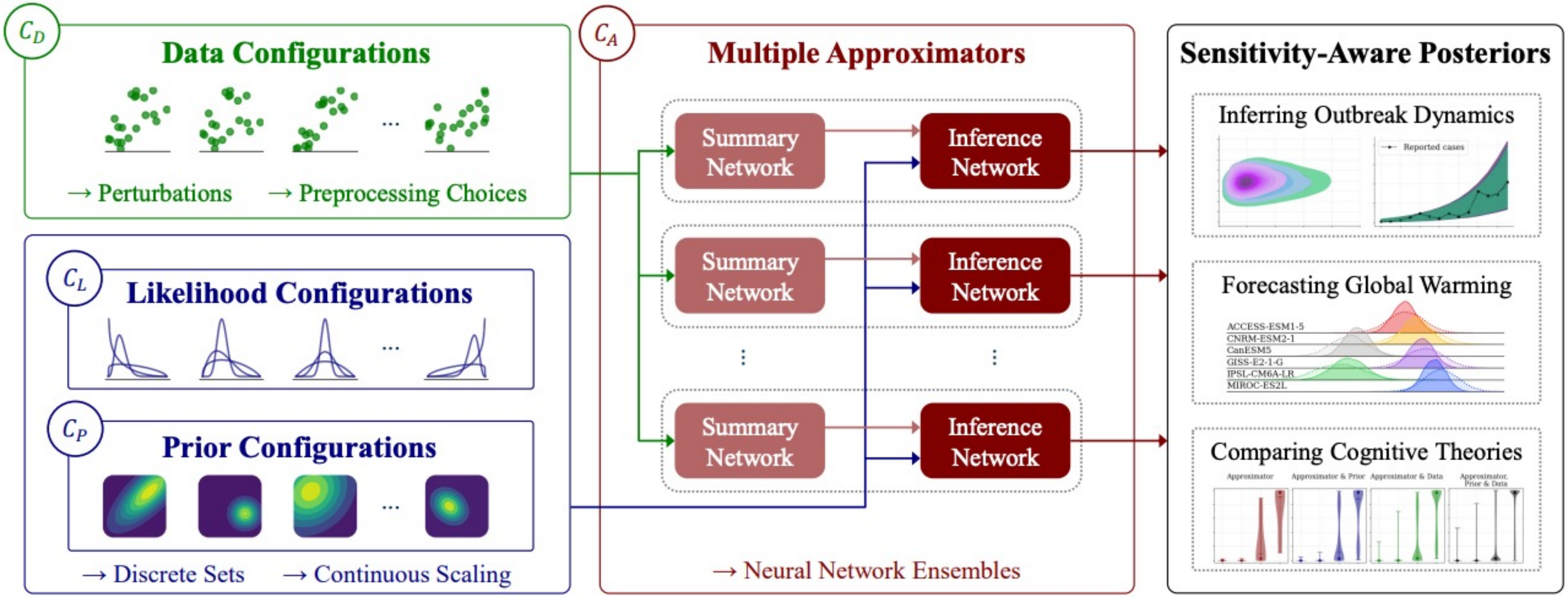
Dynamic Hierarchical Modeling





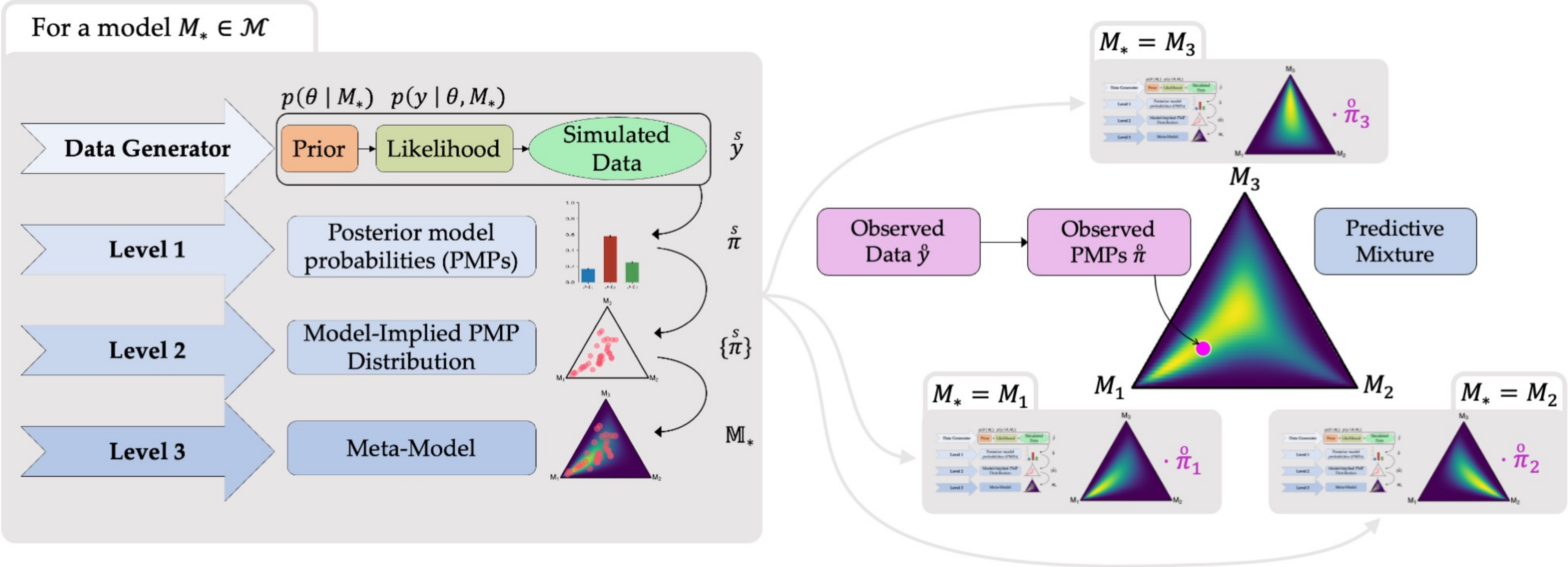
 https://arxiv.org/abs/2211.13165

Amortized sensitivity analyses



https://arxiv.org/abs/2310.11122

Meta-Uncertainty in Bayesian Model Comparison



https://arxiv.org/abs/2210.07278

Key Challenges of ABI

- Neural networks have a bad user experience
- Heaps of simulated training data necessary
- Constrained neural network architecture of normalizing flows
- Model misspecification invalidates simulation-based training

ABI library: BayesFlow

BayesFlow

Tests passing | License MIT | JOSS 10.21105/joss.05702 | contributions welcome

Welcome to our BayesFlow library for efficient simulation-based Bayesian workflows! Our library enables users to create specialized neural networks for *amortized Bayesian inference*, which repay users with rapid statistical inference after a potentially longer simulation-based training phase.

BayesFlow

Installation

```
pip install bayesflow
```

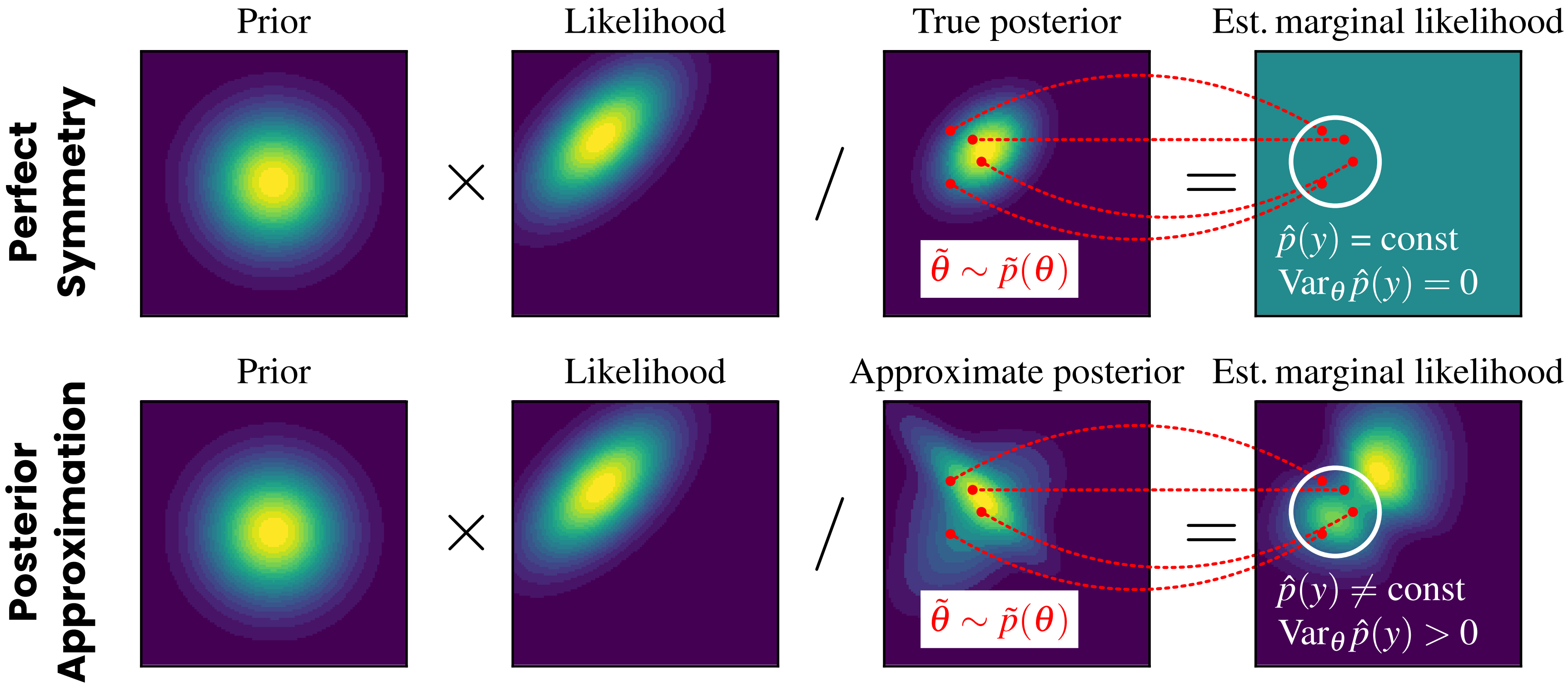
Documentation + Support

- www.bayesflow.org
- discuss.bayesflow.org

https://arxiv.org/abs/2306.16015

Low data → self-consistency

$$\boxed{p(y) = p(\theta)\, p(y \,|\, \theta) / p(\theta \,|\, y)} \implies \boxed{\frac{p(\tilde{\theta}_1)\, p(y \,|\, \tilde{\theta}_1)}{p(\tilde{\theta}_1 \,|\, y)} = \ldots = \frac{p(\tilde{\theta}_K)\, p(y \,|\, \tilde{\theta}_K)}{p(\tilde{\theta}_K \,|\, y)} \quad \tilde{\theta}_1, \ldots, \tilde{\theta}_K \in \Theta}$$



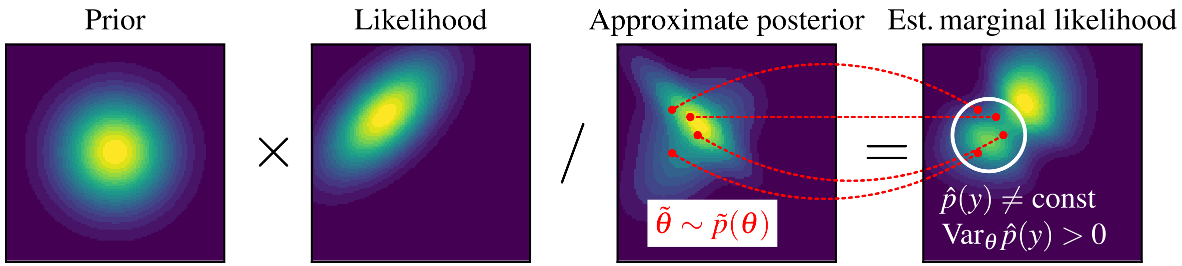
Low data → self-consistency

- **Idea:** Violations of self-consistency property as loss function

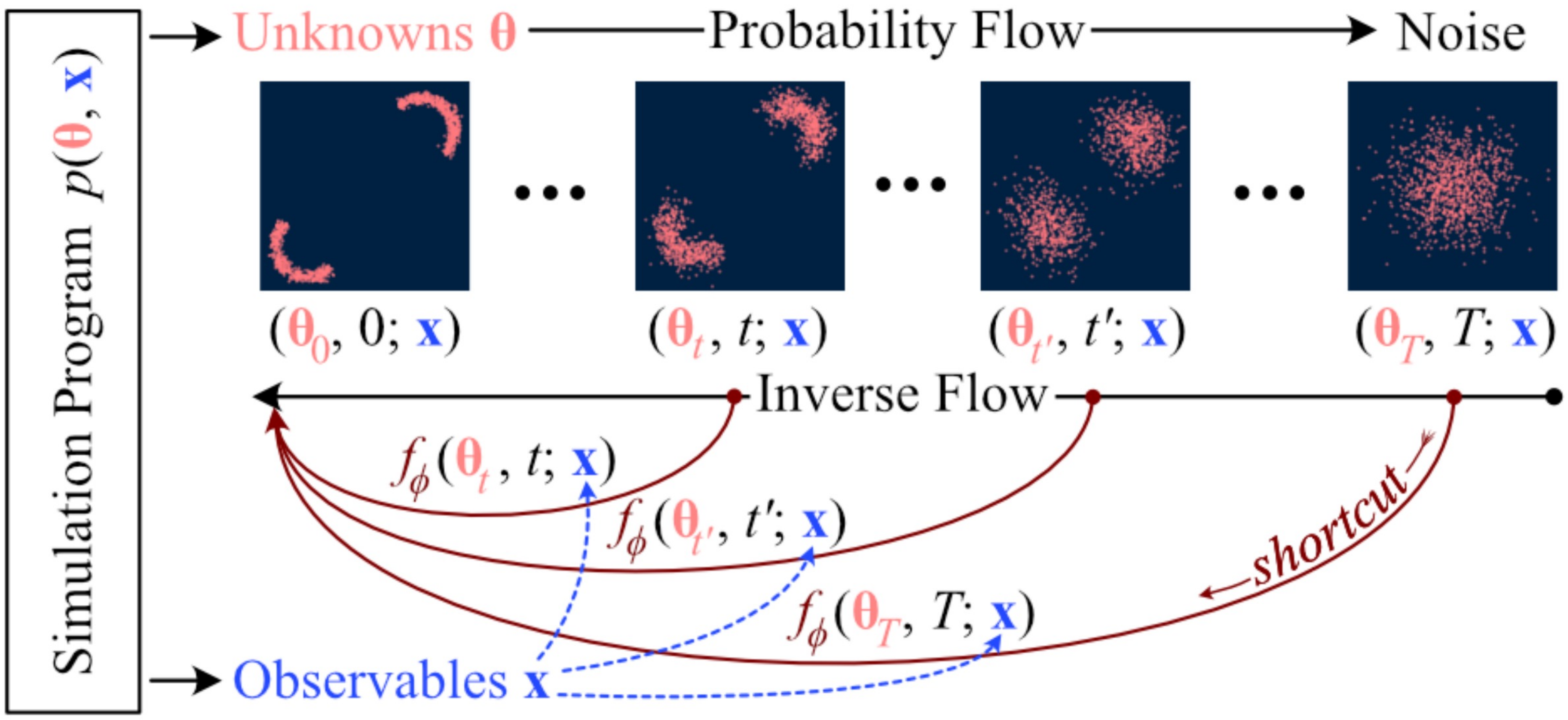
$$\mathcal{L}_{\text{SC}} := \mathbb{E}_{p(y)}\left[\operatorname{Var}_{\tilde{\theta}\sim\tilde{p}(\theta)}\left(\log p(\tilde{\theta}) + \log p(y \mid \tilde{\theta}) - \log q_\phi(\tilde{\theta} \mid y)\right)\right]$$

- **Integration** into standard neural posterior estimation loss

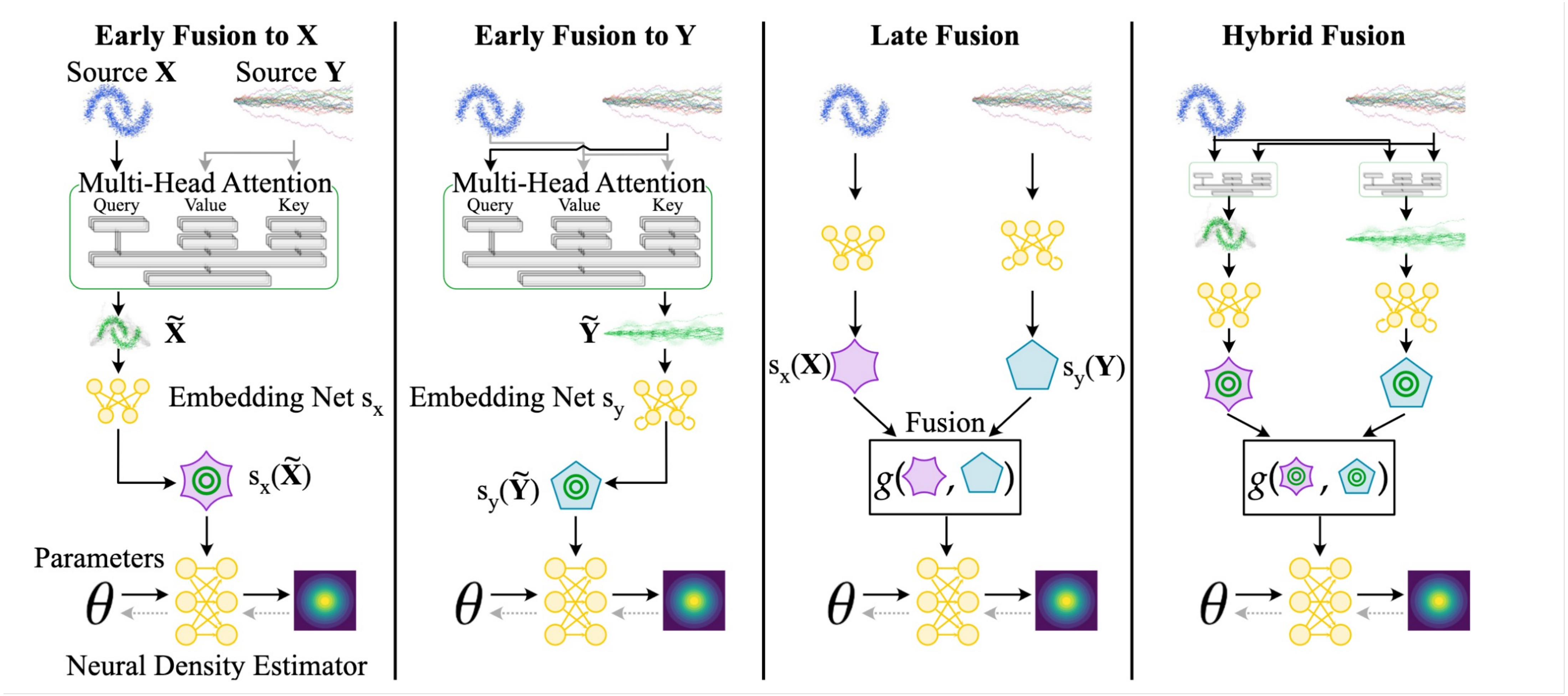
$$\mathcal{L}_{\text{NPE-SC}} := \mathbb{E}_{p(y)}\Bigg[\underbrace{\mathbb{E}_{p(\theta \mid y)}\left[-\log q_\phi(\theta \mid y)\right]}_{\text{NPE loss}} + \underbrace{\lambda \operatorname{Var}_{\tilde{\theta}\sim\tilde{p}(\theta)}\left(\log p(\tilde{\theta}) + \log p(y \mid \tilde{\theta}) - \log q_\phi(\tilde{\theta} \mid y)\right)}_{\text{self-consistency loss } \mathcal{L}_{\text{SC}} \text{ with weight } \lambda\in\mathbb{R}_+}\Bigg]$$



Neural network constraints → consistency models

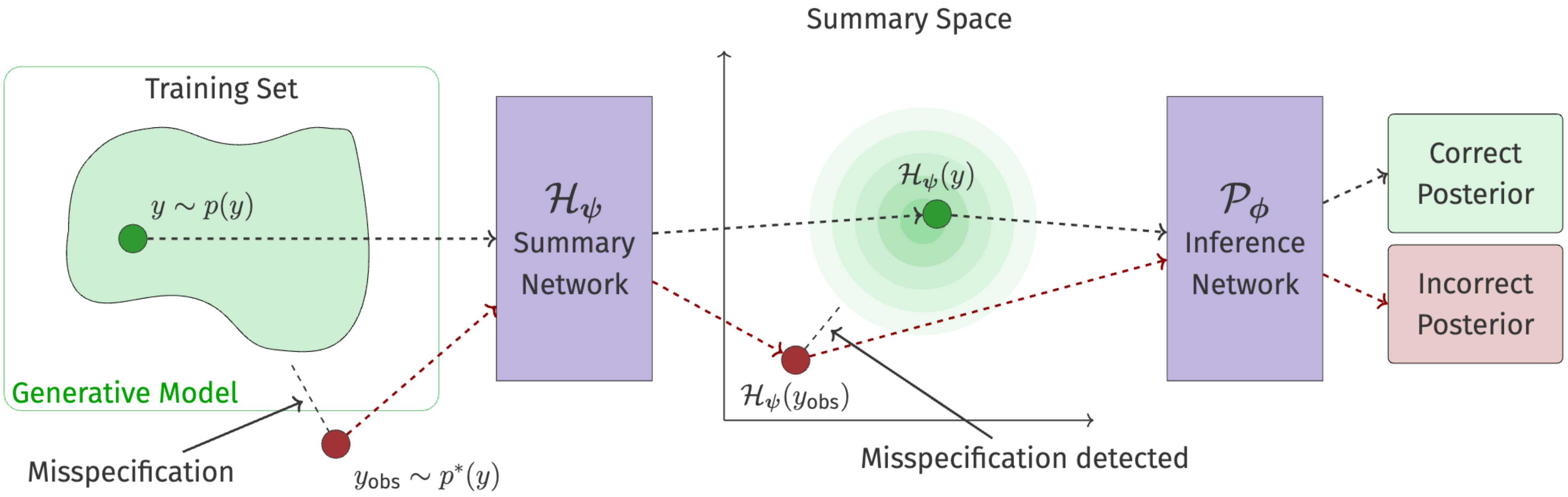


Fusing heterogeneous data sources

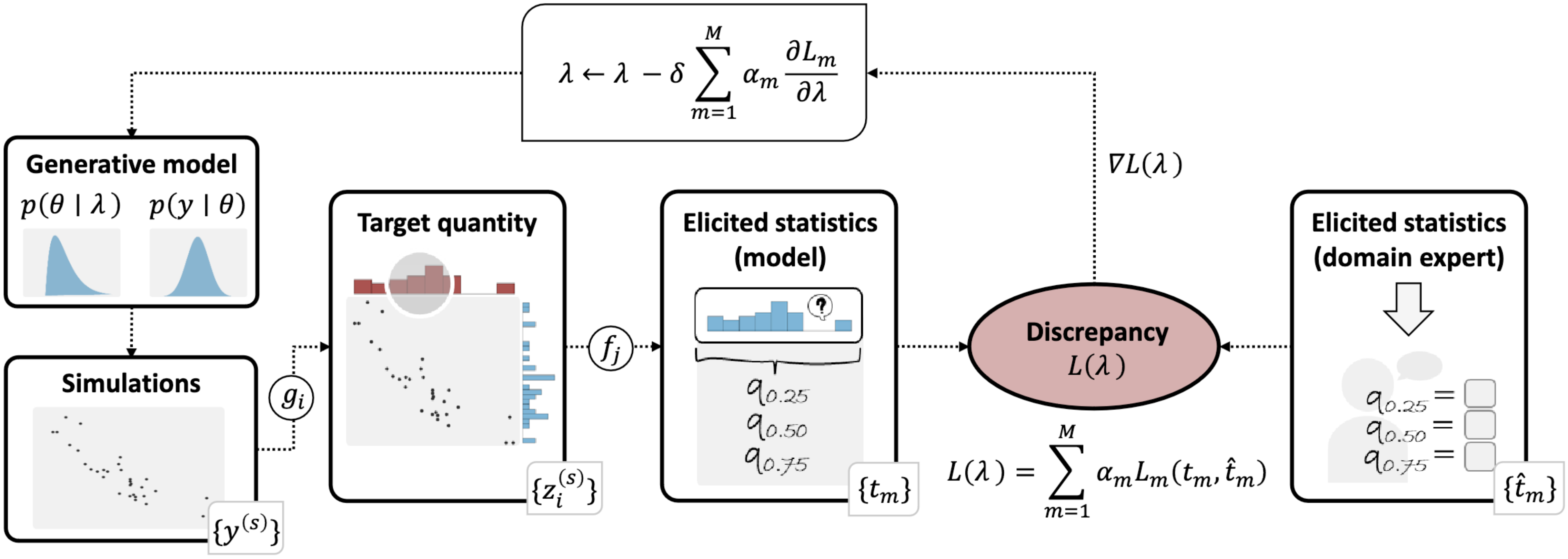


https://arxiv.org/abs/2311.10671

Model misspecification → detection



Simulation-Based Prior Elicitation



Summary

Amortized Bayesian inference

- High potential for large scale applicability
- Biggest issues: Reliability and trustworthiness
- Some questions have been tackled
- A lot of questions remain open

If you are interested in working with us, please reach out!